

**FINAL REPORT**  
**CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM**  
**CONTRACT NO. F49620-95-C-0026**

**PERIOD OF PERFORMANCE: 3/1/99 - 2/29/00**

**Prepared For:**  
**AIR FORCE OFFICE OF SCIENTIFIC RESEARCH**  
**CHEMISTRY AND LIFE SCIENCES DIRECTORATE**

**Dr. Genevieve Haddad, Program Manager**

**Presented By:**  
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**Dayton, OH 45432-1894**

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13. ABSTRACT (Maximum 200 words)  During the performance of this contract UES, Inc. provided research evaluations services for the Chemistry and Life Sciences Directorate, Air Force Office of Scientific Research in the areas of Polymer Chemistry, Surface Science, Theoretical Chemistry, Molecular Dynamics, Chronobiology and Neural Adaptation, Perception and Cognition, Sensory Systems and Toxic Biological Interactions. Evaluations were secured for 506 AFOSR Grant Proposals. UES provided administrative tasks for following meeting functions: Twenty-one program reviews - 1 in the area of Chronobiology and Neural Adaptation; 9 in the area of Surface Science; 5 in the areas of Molecular Dynamics and Theoretical Chemistry; 3 in area of Polymer Chemistry; 3 in the area of Toxic Biological Interactions. Twelve workshops were held; 3 in the area of Chronobiology and Neural Adaptation; 3 in the area of Polymer Chemistry. Thirteen panel meetings were held; 8 in Molecular Dynamics and Theoretical Chemistry; 4 in Polymer Chemistry and 1 in the area of Chronobiology and Neural Adaptation.					
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## **INTRODUCTION**

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The fourth option year effort included: 68 Proposals that were reviewed; 5 Program/Contractor Reviews; 3 Workshops and 1 Scientific Panel Meeting.

### **A. Evaluations of Individual Research Proposals**

UES sent out 67 proposals to 206 evaluators during the performance period of 1 March 1999 through 29 February 2000.

UES has been providing to the Directorate of Chemistry and Life Sciences a Summary of Proposals under Review (SPUR) report electronically on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the AFOSR Program Managers to have a current listing of all proposal activity.

### **B. Contractor/Program Reviews**

1. The first contractors review entitled **High Energy Density Matter (HEDM)** was held 8 June through 10 June 1999 at the Holiday Inn Cocoa Beach, Cocoa Beach, FL. The main purpose of this program is to research and develop advanced propellants containing increased energy densities to produce greater specific impulse, which will enable significantly increased payloads for rockets and missiles. With these advanced propellants, future space-bound payloads could be potentially four times greater than those of current systems for the same overall size and weight. UES provided on-site support, abstract booklets and made all arrangements for the meeting. There were 70 in attendance of which 28 were speakers. The proceedings from this contractors review were compiled and published and distributed by UES.

*Dr. Michael R. Berman, Program Manger*

**B. Contractor/Program Reviews – continued**

2. The first program review entitled **Tribology Program Review** was held on 14-18 June 1999 at Cheeca Lodge, Islamorada, FL. This was a joint meeting with AFOSR, the Office of Naval Research (ONR) and the National Science Foundation (NSF). The tribochemistry program is designed to provide the Air Force with improved novel lubricants, lubrication systems, and wear-resistant coatings for current-and future-generation aircraft engines. UES provided on site support, abstract booklets and made all arrangements for the meeting. The number in attendance was 56 of which 46 gave presentations. UES provided travel and per diem for one advisor to attend.

*Major Hugh De Long, Program Manager*

3. The second program review entitled **Corrosion Review** was held on 30 January through 3 February 2000 at Hawk's Cay, Duck Key, FL. This program is designed to assist the Air Force meet their requirements beyond the year 2000, the establishment of a new coatings systems, with high performance, environmentally benign corrosion inhibitors in the conversion coating or primer is needed. There were 54 in attendance of which 34 were speakers. Travel and per diem was provided by UES for two advisors to attend. UES provided abstract booklets, on-site support and handled all arrangements for this review.

*Major Paul Trulove, Program Manager*

4. The fourth program review entitled **4<sup>th</sup> Annual Review of AFOSR MURI "Nanoscale Devices and Novel Engineered Materials"** was held on 4 February 2000 at Hawk's Cay, Duck Key, FL. Twelve speakers gave presentations in this area of research. UES provided on-site support and all arrangements for this review.

*Major Paul Trulove, Program Manager*

5. The **AFOSR/ONR Electrochemistry Science & Technology Review** was held 14-16 February 2000 at the Radisson Hotel, Alexandria VA. The electrochemistry program involves molten salt systems for compact power sources and new alloy systems for a variety of Air Force systems. Specifically, to understand structure property relationships for future materials needs. thin magnetic and alloy film growth kinetics and mechanisms at the surface to understand structure property relationships for future material needs. There were 55 in attendance of which 46 were speakers. UES provided on-site support and handled all arrangements for this review. Travel and per diem was provided to one advisor to attend this program review.

*Major Paul Trulove, Program Manager*

**C. Workshops**

1. The **Human Effects Workshop** was held in Mesa, Arizona on 26-27 April 1999. Thirteen advisors made a site visit to the Williams Gateway Airport on 26 April and then convened at the Arizona Golf Resort and Conference Center on 27 April 2000. UES provided travel and per diem for 12 advisors to attend.

*Dr. Willard Larkin, Program Manager*

C. **Workshops** - continued

2. On 27-28 May 1999 a workshop on **Polymer Composites** was held at the Hyatt Regency, Long Beach, CA. There were 17 in attendance. UES provided meeting space and audiovisual equipment. Seven advisors were provided travel and per diem to attend the workshop by UES.

*Dr. Charles Lee, Program Manager*

3. The Defense Advanced Research Projects Agency (DARPA) held a workshop on their HEDM program entitled **1999 DARPA HEDM Workshop**. The workshop was held at the Holiday Inn Cocoa Beach, Cocoa Beach, FL, 11 June 1999. UES provided on-site support and meeting site.

*Dr. Michael R. Berman, Program Manager*

D. **Scientific Panel Meeting**

The **Molecular Dynamics/Theoretical Chemistry Panel Meeting** was held 3 June 1999 at the Embassy Suites Alexandria, Alexandria, VA. UES secured 31 reviewers for the 11 proposals reviewed. Abstract booklets, meeting space and audio visual equipment rental was arranged by UES. Six panel members were provided with honorarium, per diem and travel.

E. **Advisors**

Melissa M. Mallis, **Chemistry and Life Sciences Directorate**, Air Force Office of Scientific Research, Arlington, VA, 31 March 1999.

Michael Jaffee, I. C. Khoo, **AFOSR MURI Meeting**, California Institute of Technology, Pasadena, CA, 8-9 April 1999

John M. Carroll, Terry Connolly, Colin G. Drury, Daniel R. Ilgen, Richard J. Jagacinski, Bonnie Elizabeth John, Kurt Kraiger, Willard Larkin, William S. Marras, Raja Parasuraman, Karlene Roberts, Kim J. Vicente, Greg L. Zacharias, **Human Effects Workshop**, Mesa, Arizona, 26-27 April 1999.

Willard Larkin, **PRET Workshop on Biomathematical Models**, Harvard University and Endicott Conference Center, Dedham, MA, 19-21 May 1999

Peter Achermann, Torbjorn Akerstedt, Alexander Borbely, David F. Dinges and Dale M. Edgar, **Workshop on Biomathematical Models**, 19-21 May 1999

Judy Chen, John C. Halpin, Brian S. Hayes, John L. Kardos, Madhu S. Madhukar, Karl Nelson and James Seferis, **Polymer Composites Workshop**, Hyatt Regency, Long Beach, CA, 24-28 May 1999

James V. Coe, Jimmie D. Doll, Bruce C. Garrett, Paul L. Houston, James M. Lisy and James J. Valentini, **Molecular Dynamic/Theoretical Chemistry Panel Meeting**, Embassy Suites, Arlington, VA, 3 June 1999

**E. Advisors - continued**

Harold Shechter, **High Energy Density Matter Program Review**, Holiday Inn Cocoa Beach, Cocoa Beach, FL, 8-11 June 99

Jorn Larsen-Basse, Steven T. Patton, Andrey A. Voevodin, **Tribology Program Review**, Cheeca Lodge, Islamorada, FL, 14-18 June 1999

Willard Larkin, **Conference on Simulation-Based Human Performance**, University of Georgia, Athens, GA, 24-27 June 1999

Willard Larkin, **US Air Force Academy and research laboratories in Colorado**, Colorado Springs, CO, 2-3 August 1999

Nancy Cooke, Randall Engle, John Jonides, Patrick Kyllonen, **AFOSR MURI Review Meeting**, George Mason University, Fairfax, VA, 28-29 October 1999

Priya Vashishta, panel meeting on **Applying Molecular & Materials Modeling**, Princeton, NJ, 16-20 January 2000 and Albuquerque, NM, 20-22 January 2000

Keiji Morokuma, panel meeting on **Applying Molecular & Materials Modeling**, Princeton, NJ, 16-20 January 2000

Hugh De Long and Patrick Hagans, **2000 Corrosion Review**, Hawk's Cay, Duck Key, FL, 30 January-4 February 2000

Robert Mantz, **AFOSR/ONR Electrochemistry Science & Technology Review**, Radisson Hotel, Alexandria, VA, 14-16 February 2000

**F. Miscellaneous**

The **Proceedings of the High Energy Density Matter (HEDM) Contractors Conference, November 1999** was compiled, published and distributed to all attendees during this reporting period.

**SUMMARY**

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Mike Livingston, Program Manager; Judith M. Flory, Program Administrator; and Ms. Ann Corbitt, Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

## LIST OF APPENDICES

- A. Breakdown of Research Proposals by Program Manager
- B. Program for AFOSR Polymer Composites Workshop, Hyatt Regency, Long Beach, CA, 28 May 1999
- C. Summary of Review, AFOSR Molecular Dynamics/Theoretical Chemistry Review Panel Meeting, Embassy Suites Alexandria, Alexandria, VA, 3 June 1999.
- D. 1999 High Energy Density Matter Contractor's Meeting, Holiday Inn Oceanfront Resort, Cocoa Beach, FL, 8-10 June 1999
- E. 1999 DARPA HEDM Workshop, Holiday Inn Oceanfront Resort, Cocoa Beach, FL, 11 June 1999
- F. AFOSR/ONR/NSF Tribology Program Review, Cheeca Lodge, Islamorada, FL, 14-18 June 1999
- G. 2000 AFOSR Corrosion Review, Hawk's Cay, Duck Key, FL, 30 January -3 February 2000
- H. 4<sup>th</sup> Annual Review of AFOSR MURI, Hawk's Cay, Duck Key, FL, 4 February 2000
- I. AFOSR/ONR Electrochemistry Science & Technology Review, Radisson Hotel, Alexandria, VA, 14-16 February 2000
- J. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/95 - 2/29/96
- K. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/96 - 2/28/97
- L. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/97 - 2/28/98
- M. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/98 - 2/28/99

## **BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER**

<u>Program Manager</u>	<u>Number of Proposals</u>
Michael Berman	14
Robert Cohn	1
Hugh De Long	9
Walter Kozumbo	4
Willard Larkin	21
Charles Lee	17
Paul Trulove	1



## AGENDA

### AFOSR Polymer Composites Workshop

28 May 1999

Hyatt Regency Long Beach  
Long Beach, CA

- 0800 Simulated Laminated Methodology for Environmental Cycling of Polymer Composites  
*James C. Seferis, University of Washington*
- 0835 The Durability Characterization of High Temperature Polymer Matrix - Carbon Fiber Composites for Future Aerospace Application  
*Roger J. Morgan, Michigan State University*
- 0910 Moisture Transport and Thermal Aging Damage Mechanisms in Polymer Matrix Composites  
*Albert F. Yee, University of Michigan*
- 0945 Break
- 1000 The Durability Characterization of High Temperature Polymer Matrix - Carbon Fiber Composites for Future Air Force Application  
*Chuk L. Leung, PolyComp Technologies, Inc.*
- 1035 Durability Characterization of High Temperature Polymer Matrix - Carbon Fiber Composites for Future Air Force Applications: Development of Constitutive Models that Include Physical and Chemical Aging  
*J. M. Caruthers, Purdue University*
- 1110 Service Environmental Durability of High Performance Polymers and Composites  
*David Curliss, AFRL/MLBC, Wright-Patterson AFB*
- 1145 Characterizing Physical Aging in Polymeric Composites  
*C. T. Sun, Purdue University*
- 1205 Lunch
- 1300 Characterization of Aging, Deformation and Failure of High-Temperature Polymer Matrix Composites  
*Isaac M. Daniel, Northwestern University*
- 1320 Lightweight Structural Materials Research at Prairie View A & M University Fast Center  
*Paul O. Biney, Prairie View A & M University Fast Center*
- 1355 Structural Foams of Improved Strength and Thermal Stability from Random-Coil and Rigid-Rod Polymers  
*Seng C. Tan, Wright Materials Research Co.,  
Jim Mark, University of Cincinnati*
- 1430 Cure Cycle Optimization to Minimize Cure Induced Stresses  
*Madhu S. Madhukar, The University of Tennessee*
- 1505 Adjourn

**SUMMARY OF REVIEWS**  
**AFOSR Molecular Dynamics/Theoretical**  
**Chemistry Review Panel Meeting**

**99-NL-080    Spectroscopy and Dynamics of Transient Energetic Species**

-Robert Continetti, University of California, San Diego

James V. Coe, The Ohio State University (A/1)

Paul L. Houston, Cornell University (A/2)

Marsha I. Lester, University of Pennsylvania (A-/2)

James M. Lisy, University of Illinois at Urbana-Champaign (A+/2)

**99-NL-084    Physical Chemistry of Energetic Nitrogen Compounds**

-Robert Coombe, University of Denver

Paul L. Houston, Cornell University (A-/2)

James J. Valentini, Columbia University (C/2)

Ralph Weston, Brookhaven National Lab (A/3)

**99-NL-085    Studies of Transition States and Cluster-Induced Reactivity via  
Negative Ion Photoelectron Spectroscopy**

-Daniel Neumark, University of California, Berkeley

Kit Bowen, Johns Hopkins University (A+/3)

James V. Coe, The Ohio State University (A+/1)

Paul L. Houston, Cornell University (A/2)

James J. Valentini, Columbia University (A/1)

**99-NL-087    Cluster Ion Beam Studies of Fundamental Dynamics Related to  
Physical Deposition**

-Scott L. Anderson, University of Utah

James V. Coe, The Ohio State University (B+/3)

James M. Lisy, University of Illinois at Urbana-Champaign (A-/4)

James J. Valentini, Columbia University (A/3)

Nicholas Winograd, Penn State University (A-/2)

**99-NL-088    Understanding Failure of Thermal Barrier Coatings from First  
Principles**

-Emily Carter, University of California, Los Angeles

Jimmie D. Doll, Brown University (A/2)

Bruce C. Garrett, Pacific Northwest National Laboratory (A/2)

Hannes Jonsson, University of Washington (B+/2)

Steven G. Louie, University of California at Berkeley (A/A-/1)

**99-NL-090    Metal Solvation and Novel Metal-Ligand Interactions in Gas Phase Clusters**

-Michael A. Duncan, University of Georgia

Peter B. Armentrout, University of Utah (B+/2)

Philip J. Brucat, University of Florida (A/1)

Paul L. Houston, Cornell University (A-/2)

James M. Lisy, University of Illinois at Urbana-Champaign (B+/1)

**99-NL-094    State-Resolved Thermal/Hyperthermal Collisional Dynamics of Atmospheric Species**

-David J. Nesbitt, University of Colorado

James V. Coe, The Ohio State University (A+/2)

Paul L. Houston, Cornell University (A+/1)

Arthur Suits, Lawrence Berkeley Laboratory (A/2)

James J. Valentini, Columbia University (B+/1)

**99-NL-097    Advanced Simulation of Metal Clusters**

-Xiao-Qian Wang, Clark Atlanta University

Jimmie D. Doll, Brown University (Wavelet Theory A,  
Applications B/2)

Bruce C. Garrett, Pacific Northwest National Laboratory (B/2)

Robert J. Harrison, Pacific Northwest National Laboratory (A/3)

William A. Shelton, Oak Ridge National Laboratory (B+/2)

**99-NL-098    Ultrafast Vibrational Spectroscopy of Energetic Materials and Energetic Mechanical Processes**

-Dana Dlott, University of Illinois

Mark Berg, University of South Carolina (A+/2)

Eric Borguet, University of Pittsburgh (A-/A-/2)

James V. Coe, The Ohio State University (A/3.5)

James J. Valentini, Columbia University (A-/2)

**99-NL-101    Heterogeneous Catalysis and Metal/Metal-Oxide Interfaces: Interactions, Reactions and Size Effects**

-Uzi Landman, Georgia Institute of Technology

Jimmie D. Doll, Brown University (A/2)

Bruce C. Garrett, Pacific Northwest National Laboratory (A/2)

Michael Klein, University of Pennsylvania (A/not available)

Steven G. Louie, University of California at Berkeley (A/1)

**99-NL-109    Oxidation Processes on Aluminum and Rhodium**

-Andrew M. Rappe, University of Pennsylvania

Jimmie D. Doll, Brown University (A/2)

Bruce C. Garrett, Pacific Northwest National Laboratory (A-/2)

Hannes Jonsson, University of Washington (A/2)

Steven G. Louie, University of California at Berkeley (A+/1)

**99-NL-143    Quantum Simulations of Low Temperature High Energy  
Density Matter**

-Gregory Voth, University of Utah

Jimmie D. Doll, Brown University (will bring review to meeting)

**1999 High Energy Density Matter Contractor's Meeting**  
**Holiday Inn Cocoa Beach Oceanfront Resort**  
**Cocoa Beach, Florida**  
**8-10 June 1999**

**Monday, 7 June 1999**

7:00 – 9:00 PM                      Registration

**Tuesday, 8 June 1999**

7:30 – 8:30 AM                      Registration/Continental Breakfast

8:30 – 9:00 AM                      Introductory Remarks  
*Dr. Michael Berman, AFOSR*

9:00 – 9:40 AM                      AFRL HEDM Research: Perspectives, Progress, and  
Directions  
*Dr. Jeffrey A. Sheehy, AFRL, Edwards AFB*

9:40 – 10:20 AM                      Cryosolid Propellants—The Last “Revolutionary” HEDM  
Concept  
*Dr. Mario E. Fajardo, AFRL, Edwards AFB*

10:20 – 10:50 AM                      *Break*

10:50 – 11:30 AM                      The Solvation of Light Metal Atoms in Liquid Helium  
Droplets  
*Dr. Giacinto Scoles, Princeton University*

11:30 AM – 12:10 PM                      Superfluidity on Molecular Scales, in Real Time  
*Dr. Vartkess Ara Apkarian, University of California, Irvine*

12:10 – 2:00 PM                      *Lunch*

2:00 – 2:40 PM                      Fundamental Insights from HEDM Studies  
*Dr. David R. Yarkony, Johns Hopkins University*

2:40 – 3:20 PM                      Spectral Theory of The Chemical Bond: General  
Formalism for Atomic Aggregates  
*Dr. Peter W. Langhoff, AFRL, Edwards AFB*

3:20 – 3:50 PM                      *Break*

**Tuesday, 8 June 1999 (Cont'd)**

- 3:50 – 4:30 PM Spectroscopic Characterization of Non-bonding Interactions of the Aluminum Atom  
*Dr. Paul J. Dagdigian, Johns Hopkins University*
- 4:30 – 5:10 PM Adiabatic and Approximate Diabatic Potential Energy Surfaces for The Weakly-Bound Al-H<sub>2</sub> Complex  
*Dr. Millard H. Alexander, University of Maryland*
- 7:30 – 9:30 PM Propulsion for Microsatellites  
*Moderator, Dr. Patrick Carrick, AFRL, Edwards AFB*  
Air Force Microsatellite Propulsion Systems  
*Dr. Ronald Spores, AFRL, Edwards AFB*  
Scaling Issues and Design Considerations for Chemical Micropropulsion Systems  
*Dr. Andrew D. Ketsdever, AFRL, Edwards AFB*  
High Performance Chemical Propulsion for Satellite Applications  
*Dr. Tom W. Hawkins, AFRL, Edwards AFB*

**Wednesday, 9 June 1999**

- 7:30 – 8:30 AM Registration/Continental Breakfast
- 8:30 – 9:10 AM Bicyclopropylidene and 1,5-Hexadiyne from Bench Scale to Pilot Scale: Problems and Solutions  
*Dr. Suresh C. Suri, AFRL, Edwards AFB*
- 9:10 – 9:50 AM New Synthetic Methodologies for Geminal Polynitroalkanes and The Chemistry of The New HEDM Family of Diazeniumdiolates  
*Dr. D. Scott Bohle, University of Wyoming*
- 9:50 – 10:30 AM New Energetics Technology  
*Dr. Robert Schmitt, SRI International*
- 10:30 – 11:00 AM *Break*
- 11:00 – 11:40 AM New Energetic Salts for Monopropellant Candidates  
*Dr. Greg Drake, AFRL, Edwards AFB*
- 11:40 AM – 12:20 PM Development of Advanced Solid Rocket Propellants Using New Energetic Ingredients  
*Dr. Michael A. Dewey, Thiokol Propulsion*

**Wednesday, 9 June 1999 (Cont'd)**

12:20 – 2:00 PM	<i>Lunch</i>
2:00 – 2:40 PM	Theory and Synthesis of New High Energy Density Materials <i>Dr. Karl O. Christe, AFRL, Edwards AFB</i>
2:40 – 3:20 PM	N <sub>2</sub> O Dimers, Trimers and Tetramers: A New Class of Potential HEDMS? <i>Dr. Rodney J. Bartlett, University of Florida</i>
3:20 – 3:50 PM	<i>Break</i>
3:50 – 4:30 PM	Study of High Energy Species Enabled by Scalable Computing <i>Dr. Mark S. Gordon, Iowa State University</i>
4:30 – 5:10 PM	Synthesis of High-Energy High-Nitrogen Heterocycles <i>Dr. Harold Shechter, The Ohio State University</i>
7:30 – 9:30 PM	Poster Session

**Thursday, 10 June 1999**

7:00 – 8:00 AM	Registration/Continental Breakfast
8:00 – 8:40 AM	Electronic Structure Calculations for Ions in Solution: Non-Empirical Models <i>Dr. Chao-Ping Hsu, University of California at Berkeley</i>
8:40 – 9:20 AM	Laser Diagnostics for Aerosol Combustion Chemistry <i>Dr. Roger E. Miller, University of North Carolina</i>
9:20 – 10:00 AM	Nonadiabatic Dynamics of Photoexcited Reactions and Solvation Effects for Fundamental Organic Reactions <i>Dr. Sharon Hammes-Schiffer, University of Notre Dame</i>
10:00 – 10:30 AM	<i>Break</i>
10:30 – 11:10 AM	Largescale Quantum Molecular Dynamics Simulations of Low Temperature High Energy Density Matter <i>Dr. Gregory A. Voth, University of Utah</i>

**Thursday, 10 June 1999 (Cont'd)**

- |                     |  |
|---------------------|--|
| 11:10 – 11:50 AM    | Ultrafast Dynamics of Energetic Materials: Towards an Understanding of Impact Sensitivity<br><i>Dr. Dana D. Dlott, University of Illinois</i>                            |
| 11:50 AM – 12:30 PM | Atomic Propellants for Aerospace Propulsion Systems: Solid Hydrogen Experiments and Vehicle Analyses<br><i>Dr. Bryan Palaszewski, NASA John H. Glenn Research Center</i> |
| 12:30 – 12:45 PM    | Closing Remarks, adjourn<br><i>Dr. Michael Berman, AFOSR</i>   |
| 1:30 – 7:00 PM      | Lunch and tours at Kennedy Space Center  |



## **1999 DARPA HEDM WORKSHOP AGENDA**

Date: 11 June 1999

Location: Holiday Inn Oceanfront Resort  
Cocoa Beach, Florida

### **Friday 11 June**

8:00 - 8:20 a.m.	Dr. Morrish, DARPA Welcome
8:20 - 8:30	Dr. Berman, AFOSR Comments
8:30 - 9:00	Dr. Bartlett, University of Florida
9:00 - 9:30	Dr. Christe, Dr. Wilson and Dr. Sheehy, Air Force Research Lab Edwards
9:30 - 10:00	Dr. Karle, NRL
10:00 - 10:30	Break
10:30 - 11:00	Dr. Oestmark, Swedish FOA
11:00 - 11:30	Dr. Lorenzana, Lawrence Livermore Nat'l Lab
11:30 - 12:00	Dr. Russled, Naval Research Lab
12:00 - 1:00	Lunch
1:00 - 1:30	Dr. Radziszewski, Colorado School of Mines
1:30 - 2:00	Dr. Funk, Los Alamos National Lab
2:00 - 2:30	Open Speaker
2:30 - 3:30	Group Discussion, Dr. Ladouceur, Moderator
3:30 - 3:45	Dr. Morrish, Concluding Remarks
3:45	Adjourn

**AFOSR/ONR/NSF Tribology Program Review**  
**Cheeca Lodge**  
**Islamorada, Florida**  
**14-18 June 1999**

**Sunday, 13 June 1999**

1800-2100     *Registration/Reception*

**Monday, 14 June 1999**

0730            *Registration/Continental Breakfast*

0800            Progress in the Surface Science of Vapor Phase Lubrication and Frictional  
Properties of Single Crystalline Surfaces  
*Andrew J. Gellman, Carnegie Mellon University*

0830            Predicting Friction for a Vapor Lubricant Film in a Concentrated Contact Based  
on Principles of Solid Mechanics  
*Nelson H. Forster, Air Force Research Laboratory*

0900            Vapor Phase Lubricants: Nanometer-Scale Mechanisms and Applications to  
Sub-Micron and Rotating Machinery  
*Jacqueline Krim, North Carolina State University*

0930            Reactivity of Phosphate Esters with Various Substrates  
*Costandy S. Saba and David W. Johnson, University of Dayton Research Institute*  
*Nelson H. Forster, Air Force Research Laboratory*

1000            *Break*

1030            Wear Behavior of Irradiated Linear Polymer in Multi-Directional  
Sliding Contacts  
*Thierry A. Blanchet and Brian R. Burroughs, Rensselaer Polytechnic Institute*

1100            Modeling the Behavior of Polymer Nanocomposites Under Shear  
*Anna C. Balazs, University of Pittsburgh*

1130            Lunch

1300            New Materials for Controlling Friction and Wear in Extreme Environments:  
Synthesis, Tribochemistry, and Friction Mechanisms  
*Jeffrey S. Zabinski, K. Strong, and P. J. John, Air Force Research Laboratory*

**Monday, 14 June 1999 (Cont'd)**

- 1330 Real-Time Raman Tribometry: Friction, Wear and Third-Body Processes en Route to Failure  
*S. D. Dvorak, Kathryn J. Wahl, and I. L. Singer, U. S. Naval Research Laboratory*
- 1400 X-Ray SFA Studies of Molecular Organization and Surface Deformations During Lubricated Sliding  
*Jacob Israelachvili, Yuval Golan, Ana Martin, Youli Li and Cyrus Safinya, University of California at Santa Barbara*
- 1430 Computer Simulation of Sliding Hydroxylated Alumina Surfaces  
*David Mann, Wayne State University*

**Tuesday, 15 June 1999**

- 0700 *Registration/Continental Breakfast*
- 0800 First-Principles Predictions of Cleavage Energies and Fracture Toughnesses, and Simulations of Crack Propagation in Polycrystalline Diamond  
*Donald W. Brenner and Olga A. Shenderova, North Carolina State University*
- 0830 Wide Temperature Range Gas-Phase Lubrication of Polished Polycrystalline Diamond Films with Molecular Oxygen for Extreme Environment MEMS Applications  
*Michael N. Gardos, Raytheon Systems Company*
- 0900 Tribology of MEMS Materials and Devices in Extreme Environments  
*Steven T. Patton, and J. S. Zabinski, Air Force Research Laboratory*
- 0930 Molecular Dynamics Investigations of the Tribology Hydrocarbon Containing Systems  
*Judith A. Harrison, United States Naval Academy*
- 1000 *Break*
- 1030 Tribological Behavior of Polished Polycrystalline  $\alpha$ -SiC in Vacuum and 0.2 Torr/3.4 Torr Partial Pressures of Oxygen for Extreme Environment MEMS Applications  
*Michael N. Gardos, Raytheon Systems Company*
- 1100 Development and Application of Ultrahigh Resolution, Chemically-Sensitive Carbon Nanotube Probes for Surface Studies  
*Charles M. Lieber, Harvard University*

**Tuesday, 15 June 1999 (Cont'd)**

- 1130        *Lunch*
- 1300        Applications of a Non-Contacting Kelvin Probe During Sliding  
*David A. Rigney, The Ohio State University*
- 1330        Kelvin Probe Measurements Applied to Bearing Diagnostics  
*Steven Danyluk and YeYuan Yang, Georgia Institute of Technology*
- 1400        Integrated Diagnostics  
*Richard S. Cowan, Georgia Institute of Technology*
- 1430        Tribochemical Diagnostics: Optical Instrumentation and Molecular Modeling  
*Dor Ben-Amotz, Purdue University*

**Wednesday, 16 June 1999**

- 0700        *Registration/Continental Breakfast*
- 0800        The Surface Chemistry and Tribology of Metal Carbides and Nitrides  
*Scott S. Perry, University of Houston,*  
*Steve Didziulis, The Aerospace Corporation*
- 0830        Enhanced Tribological Properties of TiN/CN<sub>x</sub> Multilayer Coatings with an  
Equiaxed Microstructure  
*Dmitry Epstein, Igor Polonsky, Leon M. Keer, Michael Graham, Monica de*  
*Mesquita Lacerda, Yu-Hsia Chen and Yip-Wah Chung, Northwestern University*
- 0900        In-Situ Studies of the Nucleation and Growth of Cubic Boron Nitride  
*E. Bengu and Laurence D. Marks, Northwestern University*
- 0930        Tribological Performance and Initial Finite Element Modeling of Reactively  
Sputtered Single and Multi-layer Chromium Nitride Thin Films  
*Suzanne L. Rohde, University of Nebraska*
- 1000        *Break*
- 1030        Formation, Characterization, and Tribological Testing of Carbon Coatings on  
Silicon Carbide Produced in Chlorine Containing Gases at High Temperature  
*D. A. Ersoy, Michael J. McNallan and Y. G. Gogotsi, University of Illinois*  
*at Chicago*

**Wednesday, 16 June 1999 (Cont'd)**

- 1100      Synthesis, Modeling and Tribological Characterization of Functionally Graded Coatings  
*Sanjay Sampath, L. Prchlik, J. Gutlebar and T. Nakamura, State University of New York*
- 1130      *Lunch*
- 1300      Sol-Gel Derived, Nanostructured Oxide Lubricant Coatings  
*Douglas J. Taylor, Stuart T. Schwab, Patrick F. Fleig, TLP, Incorporated Richard A. Page, Southwest Research Institute*
- 1330      Surface Micromapping and Self-Assembling Nanocomposite Molecular Lubricants  
*Vladimir V. Tsukruk, Iowa State University*
- 1400      Characterization and Wear Mechanisms of Carbide/Carbon/Dichalcogenide Nanocomposites for Aerospace Tribology  
*Andrey A. Voevodin and J. S. Zabinski, Air Force Research Laboratory*
- 1430      Nanotribological Studies of Bulk Ceramic Materials, Multilayered Thin Films, and Liquid Lubricant Films  
*Bharat Bhushan, (Sriram Sundararajan presenting), The Ohio State University*

**Thursday, 17 June 1999**

- 0700      *Registration/Continental Breakfast*
- 0800      Efficient Parallel Algorithms for Molecular Dynamics Simulations Using Variable Charge Transfer Electrostatic Potentials  
*John W. Mintmire, U. S. Naval Research Laboratory*
- 0830      Robust Variational Fitting and Integral Factorization: Variational Divide and Conquer Density-Functional Theory  
*Brett I. Dunlap, Naval Research Laboratory*
- 0900      Chemical-Mechanical Polishing Aided by Electrical Fields  
*Steven Danyluk, Georgia Institute of Technology, Dae Soon Lim, Korea University*
- 0930      Tribochemical Polishing of Silicon Nitride and Carbide  
*Traugott E. Fischer, V. Muratov and Z. Zhu, Stevens Institute of Technology*
- 1000      *Break*

**Thursday, 17 June 1999 (Cont'd)**

- 1030 Consequences of Simultaneous Mechanical and Chemical Stimuli at Tribological and Adhesive Interfaces  
*Tom Dickinson, Washington State University*
- 1100 Ruby Coatings for Tribological Systems  
*Ursula J. Gibson, Dartmouth College*
- 1130 *Lunch*
- 1300 Correlation Between Macroscopic Forces and Molecular Orientation: A Study of Ultrathin Organic Layers by Second Harmonic Generation (SHG)  
*F. Eisert, A. Legant, M. Gurka, Manfred Buck, M. Grunze, Lehrstuhl für Angewandte Physikalische Chemie*
- 1330 Vibration Characteristics of PZT Glide Heads  
*Jin-Hui Ouyang and I. Y. (Steve) Shen, University of Washington, Alex Yl. Tasay, Castlewood Systems, Inc.*
- 1400 Electrostatic Monitoring of Wear in Oil Lubricated Contacts  
*Robert J. K. Wood, University of Southampton*
- 1430 Investigation of Multiphase Nano-Structured Carbide Coatings for Rolling Contact Applications  
*James E. Krzanowski, University of New Hampshire*

**Friday, 18 June 1999**

- 0700 *Registration/Continental Breakfast*
- 0800 Analysis of Lip Seal Behavior Using A Mixed Soft Elastohydrodynamic Lubrication Model  
*Fanghui Shi and Richard F. Salant, Georgia Institute of Technology*
- 0830 Friction Study of Carbon Nanotubes  
*David T. Shaw and Yan Chen, SUNY at Buffalo*
- 0900 Soft Configuration Model for Wearless Sliding Friction  
*Alexander L. Burin, Alexander Z. Patashinskii and Mark A. Ratner, Northwestern University*
- 0930 An Investigation of Certain Dynamic Instabilities in Dry Sliding  
*George G. Adams, Northeastern University*

**Friday, 18 June 1999 (Cont'd)**

- |      |   |
|------|---|
| 1000 | <i>Break</i>  |
| 1030 | Exploration of Tribological Coatings for MEMS Devices<br><i>Gouri Radhakrishnan, The Aerospace Corporation</i>        |
| 1100 | Topics in Tribology of Manufacturing Operations<br><i>Steven R. Schmid, University of Notre Dame</i>                  |
| 1130 | Thermal-Tribological Designs and Studies of Tribological Contacts<br><i>Qian (Jane) Wang, Northwestern University</i> |

2000 AFOSR Corrosion Review  
Hawk's Cay Resort  
Duck Key, FL

30 January – 3 February 2000

**Sunday, 30 January 2000**

1800 – 2000 Registration/Reception

**Monday, 31 January 2000**

0730 – 0800 Registration/Continental Breakfast

0800 – 0810 Welcoming and Introduction  
*P. Trulove, Air Force Office of Scientific Research*

0810 – 0820 Coatings and Corrosion Protection Task – Overview  
*M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH*

0820 – 0845 Novel Surface Preparation and Treatment Studies  
*M.S. Donley, A.J. Vreugdenhil<sup>1</sup>, V.N. Balbyshev<sup>2</sup>, M. Khobaib<sup>1</sup>, N.V. Voevodin<sup>1</sup>,  
G.A. Pacinda<sup>1</sup>, R.H. Parkhill, L.A. Kasten<sup>1</sup>, and J.T. Grant<sup>1</sup>, Air Force Research  
Laboratory, Wright-Patterson AFB, OH, <sup>1</sup>University of Dayton Research Institute,  
<sup>2</sup>Universal Technology Corporation,*

0845 – 0905 Characterization of a Novel Silicon Sol-Gel Chemistry for Al2024T3 Protection  
*A.J. Vreugdenhil, V.N. Balbyshev, and M.S. Donley, Air Force Research Laboratory,  
Wright-Patterson AFB, OH*

0905 – 0925 Electrochemical Investigation of a Silicon Sol-Gel Treatment of Al 2024-T3  
*V.N. Balbyshev and M.S. Donley, Air Force Research Laboratory,  
Wright-Patterson AFB, OH*

0925 – 0950 Organic Corrosion Inhibitors for Al 2024-T3  
*M. Khobaib and M.S. Donley, Air Force Research Laboratory,  
Wright-Patterson AFB, OH*

0950 – 1000 Coatings and Corrosion Protection Task – Summary  
*M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH*

1000 – 1015 *Break*

1015 – 1045 Measurement of Localized Corrosion Propagation Rates in Al and Al Alloys  
*G.S. Frankel, Fontana Corrosion Center, The Ohio State University, Columbus, OH*

1045 – 1115 Oxidation and Corrosion Passivation of Aluminum Surfaces  
*J.T. Yates, University of Pittsburgh, Pittsburgh, PA*



**Monday, 31 January 2000 (Cont'd)**

- 1115 – 1145 Selective Chemical Etching of Cu-Rich and Fe-Rich Inclusions from the Surface of Aluminum AA 2024-T3 Alloy  
*D. Buttry, Department of Chemistry, University of Wyoming, Laramie, WY*
- 1145 – 1315 *Lunch*
- 1315 – 1345 Nondestructive Characterization of Pitting Corrosion Damage  
*S.I. Rokhlin, The Ohio State University, Columbus, OH*
- 1345 – 1415 The Role of Coating and Substrate Heterogeneities in the Long Term Performance of Painted Aluminum Alloys: Local Detection and Mapping of Coating Defects  
*S.R. Taylor and A.M. Mierisch, Center for Electrochemical Science and Engineering, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA*
- 1415 – 1445 The Role(s) of Substrate Alloy Heterogeneity in the Corrosion of Painted Aluminum Alloys  
*J.R. Scully and G.O. Ilevbare, Center for Electrochemical Science and Engineering, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA*
- 1445 – 1515 Influence of the Bulk Solution Composition on the Blister Formation of AA2024  
*O. Schneider and R.G. Kelly, Center for Electrochemical Science and Engineering, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA*

**Tuesday, 1 February 2000**

- 0730 – 0800 *Continental Breakfast*
- 0800 – 0840 The Development of an Environmentally Compliant Corrosion Resistant and Electrically Conductive Corrosion Coating for Aluminum  
*S.R. Taylor, R.B. Leggat, and E. Pehovaz, University of Virginia, R.G. Buchheit, W. Zhang, M. Babu, A. Sehgal, L. Flores, and V. Laget, The Ohio State University, T. Gaddy, M. Josefowicz, and P. Patel, Clariant Corporation*
- 0840 – 0905 Self-Healing in Chromate-Free Conversion Coatings  
*R.G. Buchheit, S.G. Mamidipally, H. Guan, P. Schmutz, V.N. Laget, The Ohio State University, Columbus, OH*
- 0905 – 0925 Critical Factors for the Transition from Chromate to Chromate-Free Corrosion Protection  
*R.G. Buchheit<sup>1</sup>, J.H. Beatty<sup>2</sup>, M.S. Donley<sup>3</sup>, G.S. Frankel<sup>1</sup>, H.L. Fraser<sup>1</sup>, and R.L. McCreery<sup>1</sup>, <sup>1</sup>The Ohio State University, <sup>2</sup>Army Research Laboratories, <sup>3</sup>Air Force Research Laboratory*
- 0925 – 0955 Development of Non-Chromated Aerospace Coatings for Military Aircraft  
*J. Stoffer, University of Missouri-Rolla, Rolla, MO*

## **Tuesday, 1 February 2000 (Cont'd)**

0955 – 1010 *Break*

1010 – 1040 Importance of Adhesion in Corrosion Protection of Aluminum Alloys  
*H. Yasuda, University of Missouri-Columbia, Columbia, MO*

1040 – 1110 Trimethylsilane Plasma Coatings on IVD Aluminum  
*J. Deffeyes, The Boeing Company, St. Louis, MO*

1110 – 1140 Environmentally Compliant Thermal Spray Coatings for Wear and Corrosion Control  
*K. Legg, Rowan Technology Group, Libertyville, IL*

1140 – 1310 *Lunch*

1310 – 1340 Advanced Corrosion Resistant Aircraft Coatings for Outer Mold Line Applications  
*J.H. Osborne, The Boeing Company, Renton, Washington*

1340 – 1410 Sol-gel Coatings with Organic Corrosion Inhibitors  
*S.F. Cogan, M.D. Gilbert, P.J. Marren, and J. Ehrlick, EIC Laboratories, Inc., Norwood, Massachusetts*  
*J.H. Osborne, D.I. Dull, The Boeing Company, Renton, Washington*

1410 – 1440 Development of Hybrid Organic-Inorganic Coatings for Aircraft Aluminum Alloys  
*E.T. Knobbe, Department of Chemistry and the Environmental Institute, Oklahoma State University, Stillwater, OK*

1440 – 1500 Electrochemical Impedance Spectroscopy Studies of a Double Strand Polyaniline Coating on Aluminum Alloys in Acidic Environments  
*R. Racicot, US Air Force Academy, CO*

### **“Discussion”**

## **Wednesday, 2 February 2000**

0730 – 0800 *Continental Breakfast*

0800 – 0840 Mechanism of Al Alloy Corrosion and the Role of Chromate Inhibitors  
*G.S. Frankel, C.R. Clayton, R.D. Granata, M.W. Kendig, H.S. Isaacs, R.L. McCreery, S. Smialowska, and M. Stratmann, The Ohio State University, Columbus, OH*

0840 – 0910 Structure and Dynamics of Chromate Films on Aluminum Aircraft Alloy Probes with Vibrational Spectroscopy  
*R.L. McCreery, The Ohio State University, Columbus, OH*

0910 – 0920 *Break*

### **Wednesday, 2 February 2000**

- 0920 – 1000 Copper Redistribution during Corrosion and Pretreatment of Aluminum Alloy 2024  
*K. Sieradzki, N. Dimitroiv, C. Droneburg, J. Mann, and M. Vukmirovic, Arizona State University, Tempe, AZ*
- 1000 – 1030 High Resolution Analytical Microstructural Analysis of Corrosion Induced Changes in Al Alloy 2024  
*R. Carpenter, Arizona State University, Tempe, AZ*
- 1030 – 1050 Redistribution of Cathodic Reaction Kinetics During Corrosion of AlCuMg Alloys  
*T.J.R. Leclerc and R.C. Newman, UMIST, Corrosion and Protection Centre, Manchester, UK*
- 1050 – 1100 *Break*
- 1100 – 1120 Current Corrosion Research Activities at the Army Research Lab  
*P.F. Buckley, Army Research Laboratory, Aberdeen Proving Ground, MD*
- 1120 – 1220 Open Discussion – Future Directions in Air Force Corrosion Research  
*D. Peeler and P. Trulove*

### **OPEN AFTERNOON**

### **Thursday, 3 February 2000**

- 0730 – 0800 *Continental Breakfast*
- 0800 – 0830 Electrochemical, Appearance, and Contact Angle, Measurements of Aircraft Coating Systems in Combined QUV/Prohesion Exposure  
*G.P. Bierwagen and J. Li, North Dakota State University, Fargo, ND*
- 0830 – 0850 Characterization of Corrosion in Coated Metal System by Electrochemical Methods  
*G.P. Bierwagen and M. Zidoune, North Dakota State University, Fargo, ND*
- 0850 – 0910 Spectroscopic Examination of Air Force Coatings Systems During Combined QUV/Prohesion Exposure  
*A. Vreugdenhil, C. Vang, and G.P. Bierwagen, North Dakota State University, Fargo, ND*
- 0910 – 0930 AFM and SEM Studies on Aircraft Coatings under Accelerated Weathering Exposure  
*X. Yang, D. Tallman, and G.P. Bierwagen, North Dakota State University, Fargo, ND*
- 0930 – 0945 *Break*
- 0945 – 1005 Scanning Vibrating Electrode Studies of Chromated Epoxy Primer and Poly(3-Octyl Pyrrole) Coatings on Steel and Aluminum  
*G.P. Bierwagen, D. Tallman, J. He, and V. Johnston, North Dakota State University, Fargo, ND*

**Thursday, 3 February 2000 (Cont'd)**

- 1005 – 1025 Studies of Conducting Polymer Poly(3-OctylPyrrole) for Corrosion Protection  
*V. Johnston and G.P. Bierwagen, North Dakota State University, Fargo, ND*
- 1025 – 1055 EIS/ENM Instrumentation Studies  
*D. Farden and G. Miramontes De Leon, North Dakota State University, Fargo, ND*
- 1055 – 1105 In Situ Detection of Corrosion: Comparison of EIS and ENM Results from Different Experimental Electrode Configurations  
*G. Miramontes, X. Wang, and G.P. Bierwagen, North Dakota State University, Fargo, ND*
- 1105 – 1125 New High Performance Polysiloxane Primers for Aluminum  
*T.E. Ready, P. Boudjouk, S. Rohlik, V. Gelling, D. Tallman, G.P. Bierwagen, North Dakota State University, Fargo, ND*
- 1125 – 1300 *Lunch*
- 1300 – 1320 Planned Studies on the Synthesis of Probe Molecules for Better Characterization of Coating Degradation  
*M. Sibi, North Dakota State University, Fargo, ND*
- 1320 – 1340 Magnesium Powder Filled Ambient-Cure Epoxy Primers for Aluminum 2024 T-3  
*G.P. Bierwagen, North Dakota State University, Fargo, ND*
- 1340 – 1405 SVET Studies of Corrosion Initiation and Progression Under Coatings  
*M. Khobaihi, A. Buchanan and M. Donley, University of Dayton Research Institute, Dayton, OH and Air Force Research Laboratory, Wright-Patterson AFB, OH*
- 1405 – 1430 Implementation of a Hidden Corrosion Detection Assessment Methodology  
*W. Hoppe, University of Dayton Research Institute, Dayton, OH*
- 1430 – 1445 A Look Back at the AF Blue Ribbon Panel  
*M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH*
- 1445 – 1545 Open Discussion – Future Directions in AF Paint and Coatings Research  
*B. Ghim and P. Trulove*
- 1545 Closing Remarks  
*P. Trulove*

**Agenda**  
**4th Annual Review of AFOSR MURI**  
**“Nanoscale Devices and Novel Engineered Materials”**  
**University of Florida**  
**Monitor: Maj. Paul Trulove, Ph.D.**

**Friday**

**February 4, 2000**

**Location: Hawk's Cay Resort, Marathon, FL**

9:00-9:20 am	Welcome and Overview; Program Goals and Achievements S.J. Pearton (MSE/UF)
9:20-9:40 am	Mechanical Properties of Nanostructured Materials S.A. Syed Asif (NRL)
9:40-9:55 am	Magnetotransport – charge, frequency and noise properties A.F. Hebard (Physics/UF)
9:55-10:30 am	Physics of Length Scales in Magnetic and Superconducting Microstructures, I.K. Schuller (Physics/UCSD)
10:30-11:00 am	Coffee Break
11:00-11:20 am	Integration of Magnetic Nanoparticles with 2-D Electron Systems S. von Molnar (Physics/FSU)
11:20-11:40 am	Nanostructure Patterning and Transport Physics F. Sharifi (Physics/UF)
11:40-12:00 am	Ion Beam Deposited GMR Materials D. Temple and G.E. McGuire (MCNC)
12:00-1:30 pm	Lunch
1:30-1:50 pm	Dry Etching of Magnetic Multilayers, S.J. Pearton (MSE/UF)
1:50-2:05 pm	Integration of Magnetic Materials and Semiconductors F. Ren (Chem. Eng./UF)
2:05-2:20 pm	Deposition and Etching of Ferromagnetic Particles in a Non Magnetic Matrix, A.C. Kummel (Chem/UCSD)
2:20-2:35 pm	Pulsed Laser Deposition of CMR Oxides, R.K. Singh (MSE/UF)
2:35-3:00 pm	Theory and Modelling of GMR, S. Hershfield (Physics/UF)
3:00-3:15 pm	Summary and Accomplishments, S.J. Pearton
3:15-3:45 pm	Discussion (all)

AFOSR/ONR Electrochemistry Science & Technology Review  
Radisson Hotel  
Alexandria, VA

14 – 16 February 2000

**Monday, 14 February 2000**

- 12:00-1:00     Registration
- 1:00-1:25     Welcoming and Introduction  
*R. Carlin, Office of Naval Research, Arlington, VA;*  
*P. Trulove, Air Force Office of Scientific Research, Arlington, VA*
- 1:25-1:50     Nanotubule Membranes – Fundamentals and Applications in Electrochemical  
Energy and Stochastic Sensing  
*C. Martin, University of Florida, Gainesville, FL*
- 1:50-2:15     Aerogel-based Batteries: En route to a 3-D Nanoscopic Battery  
*D. Rolison, Naval Research Laboratory, Washington, DC*
- 2:15-2:40     Electrochemical Properties of Sol-Gel Derived Materials  
*B. Dunn, UCLA, Los Angeles, CA*
- 2:40-2:55     *Break*
- 2:55-3:20     Charge Transfer Systems of Molecular Dimensions  
*R. Murray, University of North Carolina, Chapel Hill, NC*
- 3:20-3:45     Dendritic- and Fractal-Based Nanotechnologies for Electrochemical Studies  
*G. Newkome, T. J. Cho, A. Mishra, C. Moorefield, G. Baker;*  
*University of South Florida, Tampa, FL*
- 3:45-4:10     Dendrimer-Encapsulated Metal Nanoparticles  
*R. Crooks, Texas A&M University, College Station, TX*
- 4:10-4:35     Extended Structures by Metal-Initiated Self-Assembly and Electrode  
Surface Structure and Composition Effects on Formic Acid Electrocatalysis  
*H. Abruña, Cornell University, Ithaca, NY*
- 4:35-5:00     Synthesis of Redox-Active and Porous Supramolecular Structures  
*M. Ward, University of Minnesota, Minneapolis, MN*
- 5:30           *Reception*

**Tuesday, 15 February 2000**

- 7:30-8:00 Continental Breakfast
- 8:30-8:55 Electron and Ion Transfer at Interfaces  
*R. Marcus, California Institute of Technology, Pasadena, CA*
- 8:55-9:20 Dip-Pen Nanolithography: A New Tool for Generating and Studying Soft Nanostructures  
*C. Mirkin, Northwestern University, Evanston IL*
- 9:20-9:45 Nanoscale Assembly of Components for Rechargeable Lithium Batteries  
*D. Sadoway, A. Mayes, MIT, Cambridge, MA*
- 9:45-10:10 Nanocomposite Polymer Electrolytes  
*E. Giannelis, Cornell University, Ithaca, NY*
- 10:10-10:25 Break
- 10:25-10:50 Ionically Conducting Channel  
*L. Scanlon, AFRL/PRPB, Wright-Patterson AFB, OH*
- 10:50-11:15 Lithiated Macrocycles in the Search for New Li-Ion Conductors  
*J. Arnold, A. Gebauer, University of California, Berkeley, CA*
- 11:15-11:40 NMR Studies of Ion Transport in Disordered Media  
*S. Greenbaum, Hunter College of the City University of New York, New York, NY*
- 11:40-12:05 Passivation Prevention Using Self-Assembled Molecular Layers at the LI/Solid Polymer Electrolyte Interface  
*D. Teeters, The University of Tulsa, Tulsa, OK*
- 12:05-1:30 Lunch
- 1:30-1:55 Combinatorial, Highly Automated and Rapid Approaches to Electrocatalyst Development  
*D. Buttry, University of Wyoming, Laramie, WY*
- 1:55-2:20 Surface Electrochemistry of Catalytic Reactions at Temperatures Ranging from Ambient to 80 °C  
*C. Korzeniewski, Texas Tech University, Lubbock, TX*
- 2:20-2:45 Development of Electrochemical Capacitor Technology for DOD Applications  
*A. Apblett, Oklahoma State University, Stillwater, OK*
- 2:45-3:10 Preparation and Characterization of Nano-structured Materials for Solid-State Electrochemical Applications  
*M. Collinson, Kansas State University, Manhattan, KS*
- 3:10-3:50 Break

## **Tuesday, 15 February 2000 (Cont'd)**

- 3:50–4:10 Electrodeposition of Transition Metal-Aluminum Alloys from Chloroaluminate Molten Salts  
*C. Hussey, University of Mississippi, University, MS*
- 4:10–4:30 The Electrodeposition of Al-Nb Alloys from Chloroaluminate Electrolytes  
*G. Stafford, National Institute of Standards and Technology, Gaithersburg, MD;*  
*G. Haarberg, Norwegian University of Science and Technology, Trondheim, Norway*
- 4:30–4:55 Studies in Buffered Chloroaluminate Ionic Liquids  
*R. Osteryoung, North Carolina State University, Raleigh, NC*
- 4:55–5:15 Ionic Liquids as Supporting Electrolytes for Supercapacitors  
*J. Stenger-Smith, Research and Technology Group, NAWCWPNS, China Lake, CA*
- 5:15–5:40 Physical Properties of the Pristine and Lithiated Substituted-Imidazolium Molten Salt Electrolytes as Liquids and as Polymer Gel Composites  
*H. De Long, U. S. Naval Academy, Annapolis, MD*

## **Wednesday, 16 February 2000**

- 7:30–8:00 Continental Breakfast
- 8:30–8:55 Electrochemistry at Nanostructured Materials: The Scaling of Molecular Transport in Small Domains  
*H. White, University of Utah, Salt Lake City, UT*
- 8:55–9:20 Fundamentals of Charge Transfer at Nanocrystalline Electrode/Solution Interfaces  
*J. Hupp, Northwestern University, Evanston, IL*
- 9:20–9:45 Influence of High Interfacial Electric Fields on the Dielectric Properties and Ionization of Water  
*E. Stuve, University of Washington, Seattle, WA*
- 9:45–10:10 Ruthenium Cluster Modification of Platinum Surfaces: Its Application on the Preparation of Pt/Ru Catalyst for Methanol Oxidation  
*C. Cabrera, University of Puerto Rico, San Juan, Puerto Rico*
- 10:10–10:25 *Break*
- 10:25–10:50 Preparation and Characterization of Thermoresponsive Polymeric Gels: Studies with Electroactive Probes  
*M. Ciszowska, Brooklyn College, Brooklyn NY*
- 10:50–11:15 Properties of Fuel Cell and Battery Materials  
*P. Stallworth, J. Fontanella, M. Wintersgill, C. Edmondson,*  
*U.S. Naval Academy, Annapolis, MD*  
*S. Greenbaum, Hunter College of the CUNY, New York, NY*



**Wednesday, 16 February 2000 (Cont'd)**

- 11:15-11:40 Modeling of On-board Fuel Cell-Based Power System for Naval Ships  
*R. White, University of South Carolina, Columbia, SC*
- 11:40-12:05 Development of Novel Electrode Materials for Use in H<sub>2</sub>S-Containing Gases  
*S. Wang, M. Liu, J. Winnick, Georgia Institute of Technology, Atlanta, GA*
- 12:05-1:30 *Lunch*
- 1:30-1:55 Development of New Fast Proton Conducting Chalcogenide Glassy Electrolytes  
*S. Martin, Iowa State University, Ames, IA*
- 1:55-2:20 Magnesium-Solution Phase Semi-Fuel Cell System Utilizing a Palladium/Iridium Catalytic Surface  
*M. Medeiros, E. Dow, Naval Undersea Warfare Center, Newport, RI,*  
*R. Bessette, University of Massachusetts Dartmouth, North Dartmouth, MA*
- 2:20-2:45 Study of Lithium Polymer Interface to Enhance Efficiency and Safety in Lithium/Water Batteries  
*M. Urquidi-Macdonald, J. Cho, Pennsylvania State University, University Park, PA*
- 2:45-3:10 Redox Cycling of Manganese on Metal Surfaces and its Consequences for Material Performance  
*Z. Lewandowski, Montana State University, Bozeman, MT*
- 3:10-3:50 *Break*
- 3:50-4:15 Thermal and Electrochemical Models for Batteries During High Rates of Discharge  
*J. Van Zee, University of South Carolina, Columbia, SC*
- 4:15-4:40 X-ray Absorption Spectroscopy and Electrochemical Studies of Novel Materials for Li-Ion Batteries  
*A. Mansour, NSWC/CD, West Bethesda, MD*
- 4:40-5:00 Conductive Polymer Moderated Reactive Metal Anodes  
*W. Ferrando, CDNSWC, West Bethesda, MD*
- 5:00 Closing Remarks/Adjourn

## APPENDIX J

**ANNUAL REPORT**  
**CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM**  
**CONTRACT NO. F49620-95-C-0026**

**PERIOD OF PERFORMANCE: 3/1/95 - 2/29/96**

**Prepared For:**  
**AIR FORCE OFFICE OF SCIENTIFIC RESEARCH**  
**CHEMISTRY AND LIFE SCIENCES DIRECTORATE**

**Dr. Genevieve Haddad, Program Manager**

**Presented By:**  
**UES, Inc.**  
**4401 Dayton-Xenia Road**  
**Dayton, OH 45432-1894**

## **INTRODUCTION**

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology; Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The first year core effort included: 132 Proposals that were reviewed; 2 Program/Contractor Reviews; 3 Workshops and 3 Scientific Panel Meetings.

### **A. Evaluations of Individual Research Proposals**

UES sent out 132 proposals to 391 evaluators during the performance period of 1 March 1995 through 29 February 1996.

UES has been providing to the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

### **B. Contractor/Program Reviews**

A total of 2 program reviews were held during this first contract year.

1. The first program review entitled **Predictive Toxicology** was held 31 May through 1 June 1995 at the Holiday Inn I-675 Conference Center, Fairborn, OH. The purpose of this meeting was to review basic research in toxicology which is supported by or of interest to the AFOSR program in Predictive Toxicology. There were 47 in attendance of which 26 were speakers that gave presentations discussing the primary objectives, results and conclusions of past research, emphasizing major accomplishments, and indicating new directions and areas of future research. The purpose of the review was to strive to achieve several goals; to inform each

research, emphasizing major accomplishments, and indicating new directions and areas of future research. The purpose of the review was to strive to achieve several goals; to inform each participant of other work being conducted under the AFOSR Toxicology Program; to exchange scientific information; to foster collaboration; and to generate new ideas. In addition, AFOSR acquired information that will facilitate technology transfers, Air Force justification of research efforts and decision-making with respect to programmatic organization.

*Dr. Walter Kozumbo, Program Manger*

2. The second program review entitled **Nonlinear Optical Polymers Contractors Review Meeting** was held on 26-28 February 1996 at the Holiday Inn I-675 Conference Center, Fairborn, OH. The purpose of this meeting was to coordinate Air Force sponsored research in this area and to promote transitions of research results to Air Force laboratories. The meeting included presentations by Air Force scientists describing potential applications for this class of materials and the desirable parameter spaces and other secondary properties necessary for these applications. Also, the Air Force applications that can potentially use nonlinear polymers and organic materials were included in this program review. The number in attendance was 104 of which 52 gave presentations.

*Dr. Charles Lee, Program Manager*

UES provided travel, per diem and honorarium for the 8 advisors who attended the Nonlinear Optical Polymers Contractors Review Meeting and then provided to AFOSR written overviews of the program reviews. UES also provided on site support, acquisition of meeting site and audio visual equipment.

### **C. Workshops**

Three workshops were held during this first year's effort.

1. On 25 May 1995 a workshop on **Environmental Effects on High Performance Polymers and Composites** was held at the Holiday Inn I-675 Conference Center, Fairborn, OH. There were 22 in attendance. UES provided meeting space and audio visual equipment.

*Dr. Charles Lee, Program Manager*

2. A workshop on **Night Operations/Human Chronobiology** was held at Bolling AFB, DC, 6-7 June 1995. UES provided travel, per diem, honorarium for the 8 advisors in attendance.

*Dr. Genevieve Haddad, Program Manager*

3. A second workshop on **Night Operations/Human Chronobiology** was held on 3-5 January 1996 at Holloman AFB, NM. There were approximately 19 attendees. UES provided travel, per diem and honorarium to 8 advisors.

*Dr. Genevieve Haddad, Program Manager*

### **D. Panel Meetings**

1. A panel meeting was held on **Atmospheric Effects of Rocket Exhaust** at the College Inn Conference Center, University of Colorado, Boulder, CO on 28 September 1995. This panel meeting of six advisors was assembled to develop knowledge necessary to assess the impact of the exhaust from rocket motors on the atmospheric environment.

2. Hanscom AFB, MA hosted a panel meeting on the **Review of Laboratory Tasks in the Molecular Dynamics Program**, 2-3 November 1995. Five advisors participated in the review of the Air Force Phillips Laboratory's program in Molecular Dynamics at Hanscom AFB, MA.

3. A panel meeting was held on **Molecular Dynamics and Theoretical Chemistry** at the Marriott's Lincolnshire Resort, Lincolnshire, IL on 30 November 1995. Seven advisors reviewed proposals in the mentioned area.

UES provided abstract booklets for all three meetings as well as on site support for the Boulder CO and Chicago IL panel meetings. Meeting space, travel, per diem and honorarium were provided for the advisors for all three panel meetings.

#### **E. Advisors**

In addition to the advisors provided for meetings, Dr. Charles Czeisler was requested to give a seminar at The Aerospace Medical Association Meeting, 7-9 May 1995 in Anaheim, CA. Dr. Czeisler also gave an overview of the meeting for AFOSR. UES provided transportation and per diem for Dr. Czeisler.

#### **SUMMARY**

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Julien M. Christensen, Program Manager; Judith M. Flory, Program Administrator; and Ms. Betty Kerans, Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

## **LIST OF APPENDICES**

Breakdown of Research Proposals by Program Manager

Program and Abstract Booklet for AFOSR Predictive Toxicology Program Review

Program for Air Force Nonlinear Optical Polymers Contractor's Review Meeting

## **BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER**

<u>PROGRAM MANAGER</u>	<u>NO OF PROPOSALS</u>
Haddad	12
Tangney	13
Lee	24
Kozumbo	25
Kroll	11
Lewis	2
DeLong	17
Hedberg	3
Berman	22
Roach	3

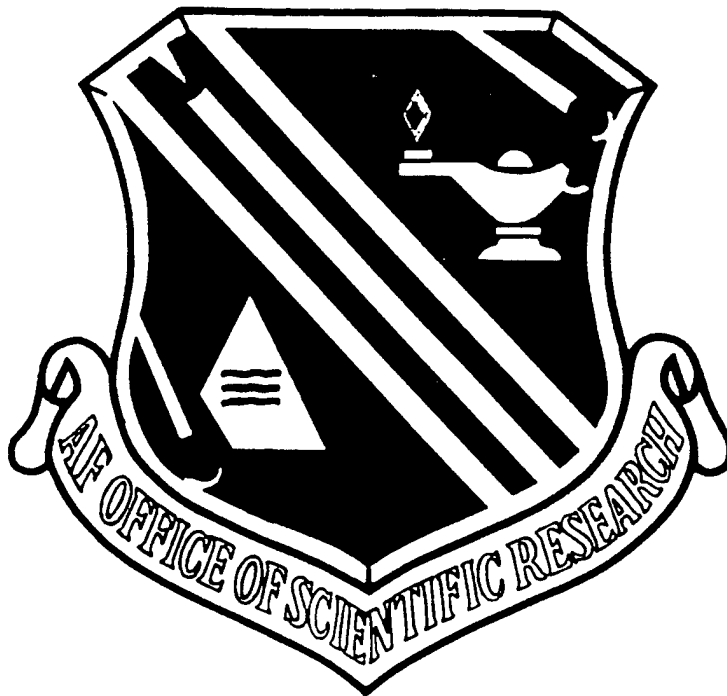


**AFOSR**

**PREDICTIVE TOXICOLOGY PROGRAM REVIEW**

**31 May - 1 June 1995**

**Holiday Inn Conference Center/I-675  
Fairborn, Ohio**



**SPEAKERS**

**Basak, Subhash  
Bernofsky, Carl  
Dallas, Cham  
Eurell, Thomas  
Harris, David  
Krishnan, Kannan  
Miller, Clay  
Myers, Charles  
Pereira, Michael**

**Reo, Nicholas  
Risby, Terence  
Robledo, Raymond  
Siegel, Frank  
Smulson, Mark  
Stohs, Sidney  
Thomas, Russell  
Trosko, James  
Witzmann, Frank**

**AFOSR PREDICTIVE TOXICOLOGY PROGRAM REVIEW**

**Walter Kozumbo, Ph.D.  
Program Manager**

**SPONSORED: AIR FORCE OFFICE OF SCIENTIFIC RESEARCH  
DIRECTORATE OF CHEMISTRY AND LIFE SCIENCES**

**UNDER CONTRACT #F49620-95-C-0026  
UES, INC.  
4401 Dayton-Xenia Road  
Dayton, OH 45432-1894**



**AFOSR PREDICTIVE TOXICOLOGY PROGRAM REVIEW**  
**Holiday Inn Conference Center/I-675**  
**Fairborn, OH**  
**31 MAY - 1 JUNE 1995**

**TUESDAY, 30 MAY 1995**

1700-1830:     \*Registration  
1830-2030:     Evening Social at Holiday Inn

**WEDNESDAY, 31 MAY 1995**

0730-0830:     Registration/Continental Breakfast

**INTRODUCTION**

0830-0845:     AFOSR and Its Program in Predictive Toxicology  
                  Dr. Walt Kozumbo, AFOSR, Bolling AFB

0845-0900:     Toxicology Program at Armstrong Laboratory/Tri-Service Toxicology  
                  Dr. Jeff Fisher, Armstrong Laboratory, WPAFB

**TOXICOLOGY AND PHARMACOKINETICS OF CHLORINATED SOLVENTS**  
(Dr. Miller as Moderator)

0900-0930:     Tools of Predictive Toxicology  
                  Dr. Clay Miller, Armstrong Laboratory, WPAFB

0930-1000:     Carcinogenic Activity of Trichloroethylene and Chloroacetic Acids In Mouse Liver  
                  Dr. Michael Pereira, Medical College of Ohio

1000-1015:     **COFFEE BREAK**

1015-1045:     Radical Intermediates of Halogenated Metabolites  
                  Dr. Carl Bernofsky, Tulane University

1045-1115:     Interspecies Extrapolations of Halocarbon Tissue Toxicokinetics  
                  Dr. Cham Dallas, University of Georgia

1115-1145:     An Interdisciplinary and Alternative Approach to Assess Carcinogenicity of  
                  Chlorobenzenes  
                  Mr. Russell Thomas/Dr. Raymond Yang, Colorado State University

1145-1300:     **LUNCHEON** at Holiday Inn

## COMPUTATIONAL TOXICOLOGY AND MODELING OF TOXIC EFFECTS

(Dr. Fisher as Moderator)

1300-1330: A Molecular Structure Based Modeling Framework for Predicting Pharmacokinetics of Organic Chemicals

Dr. Kannan Krishnan, University of Montreal

1330-1400: Use of Molecular Similarity Methods in the Risk Assessment of Chemicals: A Study with Quadricyclane

Dr. Subhash Basak, University of Minnesota

## MECHANISTICALLY BASED TOXICOLOGY

(Dr. Channel as Moderator)

1400-1430: Mechanisms Associated with the Toxicity of Polyhalogenated Cyclic Hydrocarbons and Heavy Metals

Dr. Sidney Stohs, Creighton University

1430-1445: **COFFEE BREAK**

1445-1515: Chromium Toxicity: Reductive Enzymes in Humans

Dr. Charles Myers, Medical College of Wisconsin

1515-1545: Oxidative Stress, Gap Junctional Communication and Epigenetic Toxicology

Dr. James Trosko, Michigan State University

1545-1615: Depletion of Nuclear Poly (ADP-ribose) Polymerase by Antisense RNA Expression: Influences on DNA Repair and Replication, Genomic Stability, and Survival of Cells to Genotoxic Agents

Dr. Mark Smulson, Georgetown University

1615: **ADJOURNMENT UNTIL TOMORROW MORNING**

**THURSDAY, 1 JUNE 1995**

0730-0830: **BREAKFAST** at Holiday Inn

## BIOMARKERS AS PREDICTORS OF TOXICITY IN VITRO AND IN VIVO

(Dr. Channel as Moderator)

0830-0900: Two-Dimensional Protein Pattern Recognition in Chemical Toxicity

Dr. Frank Witzmann, Indiana Univ.-Purdue Univ. at Columbus

0900-0930: A Mechanistically Based, In Vitro Evaluation of Ocular Irritants

Dr. Thomas Eurell, University of Illinois at Urbana - Champaign

0930-1000: NMR Spectroscopy as a Tool For Studies of Hepatotoxicity In Vivo

Dr. Nicholas Reo, Wright State University

1000-1030: Biomarker Analysis of Human Breath for Early Prediction of Hepatotoxicity

Dr. Terence Risby, Johns Hopkins University

1030-1045: **COFFEE BREAK**

**TOXICOLOGY OF JP-8 JET FUEL**

(Dr. Fisher as Moderator)

1045-1115     The Chronic Effects of JP-8 Jet Fuel Exposure  
                 Mr. Ray Robledo/Dr. Mark Witten, University of Arizona

1115-1145:   Immunotoxicology of Exposure to JP-8 Jet Fuel and Halogenated Hydrocarbons  
                 Dr. David Harris, University of Arizona

1145-1215:   Detoxication Enzymes as Biomarkers of Toxin Exposure  
                 Dr. Frank Siegel/Dr. Steve Kornguth, University of Wisconsin

1215-1245:   **OPEN DISCUSSION**

1245-1300:   Concluding Remarks (Walt Kozumbo) and Toxicology Program suggestions by participants

\*Registered speakers and other active participants are kindly requested not to leave until the meeting has concluded.

MILLER  
Dr. Clay R. Miller

## TOOLS OF PREDICTIVE TOXICOLOGY

Military operations require the use of numerous chemical compounds and materials. Many of these are unique to the military environment, with little information about their potential impact on the health of ground personnel or crew. Our work involves two lines of research. In the first, we have developed and validated mechanistically based assays to suggest the mechanism of toxic injury for the prototype high energy propellant, ammonium dinitramide (ADN). Using a novel reporter-gene construct linked to DNA promotion regulatory elements, we determined ADN's ability to alter cellular redox state. This suggested ADN would be an acute cytotoxicant with potential to interact with DNA. Electron paramagnetic resonance (EPR) studies demonstrated the radical products potentially produced from ADN biometabolism. The results suggested ADN to have a potential for mutagenicity. This potential was confirmed in a novel yeast translocation system and in a standard "Ames" battery. In a second line of research we have developed a pharmacodynamic (PD) model describing the mathematical dose-response for an acute biological event, lipid peroxidation. Ongoing studies using known positive compounds will be used to calibrate radical production as measured by EPR. Once validated, the PD model may serve as a template to predict similar biological effects of chemicals with no mechanistic toxicity data.

PEREIRA  
Dr. Michael A. Pereira

## CARCINOGENIC ACTIVITY OF TRICHLOROETHYLENE AND CHLOROACETIC ACIDS IN MOUSE LIVER

Trichloroethylene is an industrial solvent and degreaser that has been extensively used by the U.S. Air Force and industry. Hazardous waste sites and groundwater have been found to be contaminated with trichloroethylene. In laboratory animals carcinogenic activity has been observed in mouse liver and lung and rat kidneys. Two major metabolites of trichloroethylene, dichloroacetic acid and trichloroacetic acid, have also been shown to be carcinogenic in mouse liver. However, both trichloroethylene and the two chloroacetic acids when assayed in genotoxic/mutagenic assays, have exerted either no activity or very weak activity. Therefore, tumor promotion has been proposed for the mechanism of trichloroethylene and its metabolites, especially in mouse liver. We have or are performing initiation-promotion bioassays for trichloroethylene and the two chloroacetic acids. Tumor promotion was observed for both dichloroacetic acid and trichloroacetic acid, however, both the dose response relationship and the characteristics of the lesions induced by the two chloroacetic acids differed. The dose response relationship for dichloroacetic acid exhibited a sharp increase between 6.67 and 20 mmol/liter, while trichloroacetic acid appeared to be linear over the range of concentrations evaluated. We are continuing to explore the dose response relationship for these chloroacetic acids and trichloroethylene, as well as to characterize the lesions and pathogenesis of the three compounds. One of our objectives is to determine whether the lesions and pathogenesis induced by dichloroacetic acid and/or trichloroacetic acid are consistent to those induced by trichloroethylene. Upon completion of these studies, we will supply a better understanding of the dose response relationship for these three compounds, as well as their mechanism of action and pathogenesis in mouse liver. This would improve and support the extrapolation of the carcinogenic results obtained in mouse liver to the estimation of the human health hazard of exposure to trichloroethylene.

BERNOFSKY  
Dr. Carl Bernofsky

## RADICAL INTERMEDIATES OF HALOGENATED METABOLITES

1,1,2-Trichloroethylene (TCE) is an industrial solvent that is widely used for degreasing metals; it is also used for adhesives, paint stripping, dry cleaning, and in the manufacture of pharmaceuticals and textiles. Because of its widespread use and often improper disposal, TCE has become a common environmental contaminant at many worksites. It is also found in ground and surface waters near most large urban areas and at many landfill locations. Public exposure occurs through contaminated waters that are ultimately used for human consumption. TCE produces hepatocellular carcinomas and lung tumors in the mouse and renal tubular adenomas and testicular tumors in the rat. However, two TCE metabolites, trichloroacetic acid (TCA) and dichloroacetic acid (DCA), which are especially potent hepatocarcinogens in mice, have been implicated in the carcinogenicity of TCE. Although these haloacetic acid metabolites of TCE are capable of forming covalent adducts with DNA, the mechanism of adduct formation is unknown. By means of spin-trapping techniques, we will test the hypothesis that TCA and DCA are converted in the liver to reactive free radical intermediates that are responsible for forming these DNA adducts. Using mouse liver hepatocytes, we will examine the formation of free radicals in two ways: 1) directly, by means of electron paramagnetic resonance spectroscopy (EPR) of the trapped radicals, and 2) indirectly, through the use of a  $^{14}\text{C}$ -labeled spin trapping agent that will be converted to a stable derivative and quantitated by means of high-pressure liquid chromatography (HPLC). The rationale for the latter approach is based on recent evidence showing that viable cells have the ability to metabolize spin adducts to EPR-silent species, which could lead to a significant underestimate of radicals that have been trapped. We will also investigate the formation of DNA adducts by means of  $^{32}\text{P}$ -postlabeling techniques, and we will determine the nature of these adducts by isolating the adducted DNA, digesting it with nucleases, and identifying the modified bases by means of HPLC and mass spectroscopy.



DALLAS  
Dr. Cham E. Dallas

## INTERSPECIES EXTRAPOLATIONS OF HALOCARBON TISSUE TOXICOKINETICS

The population of the U.S. is exposed to halocarbons occupationally and in the proximity of hazardous waste sites, as well as in ambient air and drinking water. Health risk assessments of such chemicals usually require extrapolating from the results of toxicity studies in animals to predict toxic effects in man. Interspecies extrapolations for halocarbons and other volatile organic compounds (VOCs) are necessary because of very limited human exposure data. Knowledge of the pharmacokinetics of a chemical provides important information that facilitates species to species extrapolations, and kinetic studies were therefore used in this project to enable the interspecies extrapolation of toxicokinetic data.

A series of experiments have been conducted to provide a pharmacokinetic data base for evaluating interspecies comparisons of the toxicokinetics of halocarbons, and for the formulation and validation of an accurate physiologically-based pharmacokinetic model. The basic experimental design has involved giving equal doses of halocarbons to rats, mice and dogs for pharmacokinetic and neurobehavioral toxicity comparisons. Perchloroethylene (PCE), tetrachloroethane (TET), trichloroethylene (TCE), and trichloroethane (TRI) have been employed as test chemicals, in order to evaluate the relative importance of the physiochemical property of volatility on the kinetics and toxicity of halocarbons. The respiratory elimination and systemic uptake of TCE, TRI and PCE has been measured in rats and compared to available human data. In order to determine the dose received in target organs and other tissues, serial samples of brain, liver, kidney, lung, heart, skeletal muscle, and adipose tissue have been taken and analyzed for halocarbon content after administration of PCE, TCE, TET, and TRI in rats, TRI in mice, and PCE and TET in dogs. In order to provide a toxicokinetic corollary with one of these target organs, the brain, a neurobehavioral operant testing system has been employed for monitoring the central nervous system effects of halocarbons. Neurobehavioral studies have been conducted following oral and inhalation exposure to PCE, and from inhalation exposure to TRI in rats and mice using the same exposure regimens as in the kinetic studies. There was a surprising similarity in exhaled breath levels for several halocarbons between rats in this project and with previously published human data. This occurred despite physiochemical differences in volatility that might have been expected to result in significant interspecies differences. Behavioral changes for equivalent exposure regimens in mice and rats did demonstrate significant interspecies differences. It was found that blood and brain deposition was related in a dose response fashion with neurobehavioral deficit, but the time course of kinetics and toxicity showed significant differences within species.

A major objective of the project has been to develop and validate a physiologically-based pharmacokinetic model for exposure to halocarbons. The direct measurement of halocarbon concentrations in exhaled breath and tissues provided an extensive data base that was highly useful in formulating and validating the model. The model has been scaled up from the rat to dog, and their ability to predict the time-course of respiratory and tissue levels in the dog evaluated. The PBPK model was capable of accurately predicting exhaled breath and blood levels in rats during and following inhalation exposure to TRI, TCE, and PCE. Of particular interest was the ability of the model to enable various degrees of accurate predictions in the seven different tissues monitored over time following halocarbon exposures. Predictions in rats and mice were fairly accurate, especially in highly perfused tissues. The first published PBPK model predictions in dogs provided in this study were less accurate, depending on the route of administration and dose employed. Therefore, the ability of the PBPK model to predict halocarbon concentrations in species of wide variation in size, for chemicals of varying degree of physicochemical properties, and over a spectrum of doses and routes of administration was demonstrated. Important interspecies differences in the kinetics and neurobehavioral toxicity of halocarbons have been determined and will be critical in determining the ultimate utility of interspecies extrapolations of toxicokinetic data for halocarbon using PBPK models.

THOMAS  
Mr. Russell Thomas  
Dr. Raymond Yang

## AN INTERDISCIPLINARY AND ALTERNATIVE APPROACH TO ASSESS CARCINOGENICITY OF CHLOROBENZENES

The long term goal of this project is to develop an interdisciplinary approach in "Predictive and Alternative Toxicology" based on the integration of mechanistic toxicology and computer-based modeling systems [i.e., physiologically based pharmacokinetic/pharmacodynamic (PBPK/PD) models] for the evaluation of the carcinogenic activity of chlorobenzenes. The proposed studies will provide a greater knowledge of the roles of cell division and cell death in relation to chemically-induced cancer through the development of biologically-based cancer models. These models will reduce uncertainty in estimating the carcinogenic risk to humans from long-term exposure to chemical carcinogens and gain headway in the arena of low-dose extrapolation.

The proposed research will focus on 4 of the 12 isomers: 1,4-dichlorobenzene, 1,2,4,5-tetrachlorobenzene, pentachlorobenzene, and hexachlorobenzene. Chlorobenzenes are uniquely suited for this project because: (1) There is extensive basic biochemical, chemical, and toxicological information available on the selected isomers; (2) Adequate carcinogenicity bioassays have only been conducted 1,4-dichlorobenzene and hexachlorobenzene with limited carcinogenicity information available on 1,2,4,5-tetrachlorobenzene, providing a unique opportunity for predicting carcinogenicity of untested isomers, in this study, pentachlorobenzene; (3) Chlorobenzenes are very important industrial chemicals and environmental pollutants and are among the priority chemicals in the Air Force Installation Restoration Program and Bioenvironmental Hazards Program.

Our approach includes: (1) Conducting a thorough pharmacokinetic evaluation of selected isomers to assess target tissue dosimetry; (2) Evaluation of the carcinogenic activity of the four chlorobenzenes in the Ito's Medium-Term Bioassay using partially hepatectomized F344 rats and diethylnitrosamine as an initiator; (3) Parallel to Ito's Bioassay, perform "model-directed" experiments to define pharmacodynamic model parameters such as cell proliferation rates within normal liver cells and preneoplastic foci, cell death rates within normal liver cells and preneoplastic foci, and changes in cell-cycle kinetics using flow-cytometry measurements; (4) Correlating localized expression of transforming growth factor  $\alpha$ , transforming growth factor  $\beta$ , and other biomarkers of cell proliferation in proliferating hepatocytes and preneoplastic nodules; (5) Integration of the above information into a PBPK/PD model to quantitatively assess the roles of cell division and cell death in relation to cancer and chlorobenzene exposure and formulate a predictive approach to assess carcinogenesis.

KRISHNAN  
Dr. Kannan Krishnan

## A MOLECULAR STRUCTURE BASED MODELING FRAMEWORK FOR PREDICTING PHARMACOKINETICS OF ORGANIC CHEMICALS

The pharmacokinetic behavior of chemicals in biota is determined by certain chemical-specific and species-specific parameters. The chemical-specific parameters primarily refer to tissue:air, blood:air and tissue:blood partition coefficients (PCs). The species-specific parameters include cardiac output, alveolar ventilation rate, tissue volumes and tissue blood flow rates. Biochemical parameters such as absorption rates, binding constants, and metabolic rate constants are both chemical- and species-dependent. Physiologically-based pharmacokinetic (PBPK) models provide a framework to integrate the interrelationships among physiological, physicochemical and biochemical parameters to provide simulations of tissue dose of chemicals. PBPK models have been developed and validated for a limited number of volatile organic chemicals. There is an urgent need to develop mechanistic, predictive methodologies for a parameterization of PBPK models, to enable the use of these models early on in the product development and risk assessment processes. The objective of the present work is to develop a molecular structure based PBPK model framework for predicting the pharmacokinetics of organic chemicals. To forecast the pharmacokinetics and tissue dosimetry of untested organic chemicals, numerical values of the PCs and biochemical constants specific to a chemical in the species of interest are required. For predicting the PCs of organic chemicals, we have developed an algorithm based on tissue and blood composition data. Accordingly, the tissue:blood PCs are estimated by accounting for the relative solubility of chemicals in the neutral lipid, phospholipid, and water fractions in tissues and blood. This approach facilitates the characterization of each tissue compartment in the PBPK model as a mixture of neutral lipids, phospholipids, and water (instead of considering the model compartments as "empty" boxes as done conventionally). This approach also enables the automated calculation of tissue:blood PCs from n-octanol and water solubility data, since these are approximated to solubility of chemicals in tissue/blood lipids and water. Using the present approach, the tissue:blood PCs could also be calculated within PBPK models by providing chemical structural information as input. Accordingly, each chemical is introduced into the model as a set of fragments (e.g., a methyl, carboxyl), each of which contributes a particular numerical value (i.e., a fragment constant) to the log n-octanol:water PC of the chemical. This datum is then used in the algorithm based on tissue and blood composition to predict tissue:blood PCs of chemicals within PBPK models. Future work in our laboratory will be directed toward the development and validation of methodologies for predicting the oral/dermal absorption constants, tissue diffusion coefficients, hemoglobin binding constants, and affinity and velocity of metabolism of organic chemicals from molecular structures. The development and validation of a modeling framework to forecast tissue dosimetry and toxicity of chemicals based on their molecular structures should enhance our ability to choose and prioritize, from the multitude of chemicals available, the relatively "safer" ones for further detailed testing and potential use.

BASAK  
Dr. Subhash C. Basak

## USE OF MOLECULAR SIMILARITY METHODS IN THE RISK ASSESSMENT OF CHEMICALS: A STUDY WITH QUADRICYCLANE

Risk assessment of chemicals is often carried out with limited or no experimental data. Frequently, no biological test data and empirical physicochemical properties necessary for hazard estimation are available. In the face of the paucity of data, the hazards posed by environmental pollutants is estimated using two major approaches; a) class specific quantitative structure-activity relationship (QSAR) models and b) structural analogs of toxicants.

In the first approach, a pollutant is assigned to a particular structural class and QSAR model for that class is used in estimating the hazard posed by the pollutant. But often a complex chemical cannot be placed into a particular class unequivocally. In such cases, the other viable alternative is to select analog(s) of the pollutant and use hazards of the **analog(s)** (or **similar chemicals**) to estimate the hazardous potential of the candidate chemical. Often the analogs are selected intuitively based on the individual judgment of the expert.

We have developed a number of methods for quantifying intermolecular similarity using nonempirical parameters. Such parameters can be calculated directly from molecular structure and can be computed for any arbitrary chemical species. Analogs are similar chemicals selected by such nonempirical techniques can be used for the hazard estimation of chemicals.

In this presentation we will discuss the development of a few molecular similarity methods. Use of quantitative molecular similarity analysis (QMSA) methods in estimating properties like boiling points, mutagenicity, octanol/water partition coefficient (logP) of various sets of molecules will be presented. We will also illustrate applications of QMSA methods in selecting analogs of quadricyclane from different and large data bases containing properties relevant to hazard assessment. Finally, we will compare relative efficacies of similarity methods vis-a-vis statistical and neural net methods in predicting properties.

STOHS  
Dr. Sidney J. Stohs

## MECHANISMS ASSOCIATED WITH THE TOXICITY OF POLYHALOGENATED CYCLIC HYDROCARBONS AND HEAVY METALS

Occupational exposure to structurally dissimilar polyhalogenated cyclic hydrocarbons (PCH) and heavy metals produce similar toxic effects including hepatotoxicity, neurotoxicity, progressive weight loss, and death. The cascade of events which occurs following exposure to these xenobiotics is not known, and therefore the mechanisms(s) of action of these toxicants has not been elucidated. Studies in our laboratories have demonstrated that PCH as lindane, TCDD, and endrin, and heavy metals as chromium and cadmium induce the production of reactive oxygen species in hepatic mitochondria and microsomes as well as peritoneal macrophages. Antioxidants/free radical scavengers can attenuate these effects. The urinary excretion of the lipid metabolites malondialdehyde, formaldehyde, acetaldehyde and acetone may be effective biomarkers of exposure to these xenobiotics. Preliminary studies have suggested that the activation of the protein kinase C second messenger system, release of the cytokine tumor necrosis factor- $\alpha$  (TNF $\alpha$ ) and induction of stress/heat shock proteins occur in response to these diverse substances. We have hypothesized that the toxic manifestations are at least in part induced through a series of events involving the production of reactive oxygen species, activation of the protein kinase C system and release of TNF $\alpha$ . The sequence of these events is not known, and the relationship between these events and the induction of stress protein has not been studied. Both in vivo and in vitro effects on these parameters will be determined. Initial studies will be conducted in rats and mice using a single, oral, acutely toxic dose equivalent to one-half the LD<sub>50</sub> to provide a baseline for subsequent studies. In vitro studies will be conducted in macrophage J774A.1 and Chinese hamster ovary cell culture systems. Since most occupational exposure involves chronic, low doses, low dose chronic studies will be conducted. Dosing for up to 120 days will be conducted using a dose in the range of 1/10th-1/100th the acute dose. Animals will be sacrificed at 15 day intervals. Initial studies will focus on the identification and quantitation of biomarkers of toxicity including the urinary excretion of the lipid peroxidation products malondialdehyde; formaldehyde, acetaldehyde and acetone by HPLC, the production of reactive oxygen species by spectroscopic methods, an increased incidence of DNA single strand breaks by alkaline elution, enhanced production of TNF $\alpha$ , activation of the protein kinase C system, and induction of stress proteins by PAGE. Selected antioxidants/free radical scavengers and membrane stabilizers will be used to evaluate the role of reactive oxygen species in the activation of protein kinase C system, production of TNF $\alpha$  and induction of stress proteins. In summary, the results will greatly contribute to our knowledge of the mechanisms of toxicity of polyhalogenated cyclic hydrocarbons and heavy metals, and whether similar mechanistic pathways are involved. Information regarding biomarkers of exposure will be obtained, and the information will be exceedingly useful in developing strategies, and protocols for preventing and treating toxicities associated with occupational exposure to these xenobiotics.

MYERS  
Dr. Charles Myers

## CHROMIUM TOXICITY: REDUCTIVE ENZYMES IN HUMANS

Chromium (Cr) compounds are in wide use as components of many industrial processes and products. Exposure to Cr compounds can occur through occupational exposure, the environment, or the domestic use of Cr-containing products. Exposure to Cr compounds is associated with a wide array of toxic effects, including ulcerations, potentially serious damage to internal organs and increased incidence of certain cancers. The reductive metabolism of Cr(VI) to Cr(III), via reactive intermediates, is thought to play a key role in the cytotoxicity, mutagenicity, and potential carcinogenicity of Cr compounds. Studies on Cr(VI) reduction in human systems are scarce, and yet this information is central to understanding Cr toxicity and the potential for Cr-induced carcinogenesis in humans.

In rodents, microsomal enzymes are one class of cellular components which can mediate Cr(VI) reduction. Preliminary studies in our lab suggest that these rodent studies do not accurately reflect microsomal Cr(VI) reduction in humans. Based on our findings, we hypothesize that human microsomal enzymes can mediate Cr(VI) reduction at significant rates, at concentrations that are physiologically relevant, and under O<sub>2</sub> tensions typical for most well-oxygenated tissues. We further hypothesize that these Cr(VI)-reducing enzymes may irreversibly bind Cr as a result of Cr(VI) reduction and that this binding may disrupt their normal enzymatic role. Finally, we hypothesize that microsomal flavoenzymes (e.g. P450 reductase and flavin-containing monooxygenase), are likely candidates as the major microsomal Cr(VI)-reducing enzymes.

The specific aims of this proposal are to examine Cr(VI) reduction by human microsomes in order to: (1) determine the general characteristics of Cr(VI) reduction by human microsomal enzymes, including determination of both the kinetic aspects of, and interindividual differences in, microsomal Cr(VI) reduction; (2) elucidate the effects of various levels of O<sub>2</sub> on human microsomal Cr(VI) reduction; (3) examine the potential irreversible binding of Cr to microsomes as a result of Cr(VI) reduction, and the potential effects of this binding on microsomal enzyme activities; and (4) determine the ability of key microsomal enzymes, including NADPH:cytochrome P450 reductase and flavin-containing monooxygenase(s), to mediate Cr(VI) reduction.

Together, these studies will provide necessary and important insight into the potential mechanisms of human microsomal Cr(VI) reduction and hence into the cytotoxicity, genotoxicity, and carcinogenicity of Cr(VI) compounds in man.

TROSKO  
Dr. James E. Trosko

## OXIDATIVE STRESS, GAP JUNCTIONAL COMMUNICATION AND EPIGENETIC TOXICOLOGY

Gap junctional intercellular communication (GJIC) is a fundamental biological process in all multicellular organisms which has been implicated in the regulation of cell proliferation, differentiation and adaptive responses of differentiated cells. Disruption of GJIC by many non-genotoxic chemicals and oncogenes has been linked to several disease endpoints, including teratogenesis, tumor promotion, reproductive and neurotoxicological dysfunctions. The goal of this proposal is to continue our studies on the mechanisms by which toxic chemicals can block GJIC, particularly those that induce oxidative stress in both human and rodent cells, in vitro and selected chemicals of interest to the AFOSR (namely tetracycloheptone, fluorocarbon ethers, and ammonium dinitramide). The specific aims will be to determine (a) if a series of known toxic chemicals can inhibit gap junctional intercellular communication (GJIC) in several human and rat cell lines; and (b) if the generation of free radical oxygen species is responsible, via some mechanism, for altering GJ function. GJIC will be measured using the scrape loading/dye-transfer fluorescent recovery after photobleaching (FRAP) and microinjection - FRAP techniques. The mechanisms by which chemicals block GJIC will be tested at the transcriptional translational and posttranslational levels using molecular biological/biochemical techniques (northern, westerns, in situ immunofluorescence) with probes for the gap junction genes and antibodies for the connexin proteins.

The test of the hypothesis that these toxic chemicals which block GJIC also block programmed cell death or apoptosis will also be made. Finally, a series of biochemical/fluorescent imaging techniques to determine the specific mechanism by which oxidative-stress inducing toxic chemicals block GJIC will be utilized. The significance of these studies will be to understand the detailed manner by which important toxic chemicals block GJIC to lead to various diseases in order that specific remediation/chemoprevention strategies can be devised. The specific experimental approach will involve various toxic chemicals (e.g., dichloroacetic acid; trichloroacetic acid; chloral; quadricyclane; chromium salts; cyanide; naphthalene; ethylene glycol; 2,6-dinitrotoluene, etc.) which will be placed on human kidney epithelial, rat liver epithelial and glial cells, at non-cytotoxic levels to determine if gap junctional intercellular communication (GJIC) will be inhibited. If any of these chemicals are found to block GJIC, various assays to determine (a) if radical oxygen species are generated (fluorescence detection with 2,7-dichlorofluorescein in the presence of selected free radical scavengers; spin trapping); (b) to determine if a change in the oxidative status of a cell results from changes in the intracellular levels of anti-oxidant mechanisms (i.e., GSH, GSH peroxidase, ascorbate,  $\alpha$ -tocopherol, catalase); (c) the potential biochemical mechanisms(s) by which free radicals inhibit



GJIC (e.g., alterations in intracellular free  $\text{Ca}^{++}$  or pH; activation of phosphorylation/de-phosphorylation of gap junction proteins, etc.). This in vitro model to study both basic mechanisms and development of protective measures can also reduce the need for animal toxicity studies. As part of these studies, comparative effects of those toxic chemicals of concern to the USAFOSR on GJIC in both human and rodent cells in vitro, as well as cells from different organs (e.g., skin, liver, brain, etc).

SMULSON  
Dr. Mark E. Smulson

DEPLETION OF NUCLEAR POLY (ADP-RIBOSE) POLYMERASE BY ANTISENSE  
RNA EXPRESSION: INFLUENCES ON DNA REPAIR AND REPLICATION,  
GENOMIC STABILITY, AND SURVIVAL OF CELLS TO GENOTOXIC AGENTS

**Poly(ADP-ribose) polymerase (PADPRP)** is a chromatin-bound enzyme which is pivotal in cellular recovery from DNA strand break damage. Three additional years of research support is requested from the AFOSR for our program which concerns, first, the use of biotechnology and molecular biology approaches towards the elucidation of the biochemical mechanisms by which this enzyme mediates repair of cells from specific **environmental toxic agents**, of interest to AFOSR and secondly, in a practical vein, to experimentally exploit the properties of this enzyme and its product, poly(ADP-ribose) to develop new **Biomarker** assays to be used in collaboration with intramural AF laboratories as a novel assessment of environmental hazards.

PADPRP requires DNA for activity, and it is significant that the catalytic activity of this enzyme is directly coordinated with the number of DNA strand breaks in DNA, both in vitro as well as in vivo. Thus, poly(ADP-ribosyl)ation is rapidly modulated in response to environmentally significant, DNA-damaging agents; it probably represents the most initial response of the cell to genotoxic damage to the genome. Accordingly, significant reductions in cellular NAD levels reflect increased poly(ADP-ribosyl)ation due to DNA strand breaks. Hence, it is of significance to this application that Proctor and Casida showed that 38 organophosphorus and methyl carbonate insecticides in doses as low as 0.6 parts per million cause lowering of NAD. The levels of NAD were directly correlated with teratogenesis in this study.

Our laboratory, during earlier AFOSR granting periods, was the first to isolate and clone a full-length cDNA for PADPRP. In subsequent years, our experiments focused on understanding how poly(ADP-ribosyl)ation affects chromatin structure overall and DNA repair and replication specifically. For these studies, we developed several biochemical and immunological techniques and assays, many of which continue to be useful in the proposed future continuation. More recently, we have also provided a variety of molecular biology techniques. One of the major aims over the past few years of this project has been to establish and characterize cells stably transfected with PADPRP antisense cDNA under the control of an inducible promoter and to establish conditions under which significant depletion of nuclear PADPRP could be achieved. This approach has been particularly successful in assessing the potential roles of poly(ADP-ribosyl)ation in a variety of biological processes, all involving DNA strand breaks, without the use of non-specific chemical inhibitors. Thus, we have assigned biochemical roles for PADPRP in the recovery of cells with exposure to mutagenic agents, gene amplification and DNA replication. These past studies should allow us to learn considerably more about the mechanism role of this enzyme in cells exposed to stressful environments, and also to the development of more practical **Biomarker** assays, coupled with this reaction.

Accordingly, in AIM I of the renewal program, we propose to exploit the experimental protocols established during the last granting period with HeLa cells transfected with PADPRP antisense RNA constructs to further study the role of this enzyme in DNA repair, strand rejoining reactions, and chromatin reassembly in other cell systems, appropriate to environmental agents of interest to AFOSR (i.e. ADN, *hydrazine*, *trichloroethylene*, *tetrochloroethylene*, *N-Nitrosodimethylamine*, and *cadmium*, etc.). For example, a novel human immortalized karytinocyte cell line transfected with antisense to PADPRP has been developed in pilot studies, since skin is one tissue at high risk to exposure to a number of environmental agents. These engineered skin tissue culture cells have been grafted onto mice and form a layer of human skin, which is histologically identical to normal skin, then, using new **Biomarker** methods, piloted in **AIM II**, we have shown that topical addition of an alkylating agent (as a prototype for other agents) elicits rapid synthesis of poly(ADP-ribose) polymer (an indirect measure of DNA breaks). Other types of cells and organs will be tested in **AIM I**. we will also determine whether sufficient PADPRP-DNA-binding domain can also be induced (in various cells) as an alternative method to inhibit endogenous nuclear polymerase activity completely.

The experiments projected in **AIM II** are a logical extension of the biology and biochemistry information gained in **AIM I**. These new approaches represent a practical utilization of this information by developing two new **Biomarker** assays for the assessment of environmental hazardous agents. Observations relevant to this aim include the following: (a) The biosynthesis of the unique biopolymer, poly(ADP-ribose) is one of the earliest responses of cells to DNA damage, as elicited by many environmental hazardous agents; (b) The DNA-binding Domain of PADPRP is among the most effective cellular proteins which binds to both single and double strand DNA breaks. Our laboratory, during the last period, has overexpressed this human protein in bacteria. We propose to develop two new **Biomarker** assays, of which preliminary data suggests a high level of feasibility. On the one hand, we will develop a bioassay using the ability of antibody, specific to poly(ADP-ribose) polymer to detect this product (and indirectly DNA damage) on fixed cells or tissues. Secondly, we will develop a similar type of assay to detect DNA strand breaks in tissues cells or tissues by the unique binding of the PADPRP-DBD on fixed slides or tissues which have been exposed to hazardous agents and subsequently the detection of this bound protein only to DNA ends by immunological procedures.

WITZMANN  
Dr. Frank A. Witzmann

## TWO-DIMENSIONAL PROTEIN PATTERN RECOGNITION IN CHEMICAL TOXICITY

The Air Force Program in Toxicology is interested in developing a more proactive approach to toxicity testing, one based on predictive toxicology. Through our interaction with the Toxicology Division of the Armstrong Laboratory and the unique capabilities we possess, our laboratory is developing a predictive toxicology based on pattern recognition. By using two-dimensional electrophoresis of proteins (2D-PAGE), we are developing methods for comparing computer-recognized 2D-protein pattern alterations in various target tissues induced by specific chemical agents to quickly, economically, and reliably assess and predict hepatotoxicity, nephrotoxicity, or immunotoxicity, etc., as well as toxic mechanism. The strength of the large-scale 2D-PAGE technique lies in its ability to resolve literally thousands of cellular proteins in a single sample, first based on their content of acidic and basic amino acids (isoelectric focusing), and second by molecular weight (SDS electrophoresis). In combination, these two separation techniques produce a two-dimensional protein pattern unique for each tissue or group of cells tested. Individual proteins within the pattern can be analyzed for alterations in volume (density), charge, and molecular weight. Changes in volume or spot density reflect alterations in a protein's abundance and suggest up- or down-regulation of the genome or altered protein turnover rates. Charge modifications suggest either postranslational modification or point mutations in the genome. Regardless of the type of changes observed, a well-resolved 2D protein pattern, or *2D protein map (fingerprint)*, provides a pattern realistically containing 1000-2000 proteins and is thus a significant source of information regarding the health/activity of a particular cell/tissue type. With the advent of user-friendly computerized imaging of the protein patterns generated by 2D-PAGE and its use in pattern recognition for animal model target tissues, 2D-PAGE has become an even more powerful technique in toxicity testing; one with increasingly well-documented potential.

EURELL  
Dr. Thomas E. Eurell

## A MECHANISTICALLY BASED, IN VITRO EVALUATION OF OCULAR IRRITANTS

There are currently more than 40 published in vitro tests for predicting the ocular irritancy potential of test substances. Although these tests range in complexity, they all share the major obstacle of validation in predicting the in vivo ocular response. Our research team has developed three dimensional, in vitro organotypic models for the rabbit and human anterior cornea which we believe will provide information necessary to address the problem of assay validation. The organotypic models (corneal equivalents) consist of a collagen-based stromal matrix which is supported by a polycarbonate membrane and contains rabbit corneal keratocytes and epithelial cells. The corneal epithelial cells are grown on top of the stromal matrix and allowed to differentiate into basal, wing and superficial epithelial layers. The resulting three dimensional models are histologically and biochemically analogous to their respective native tissues.

Tissue isoelectric focusing (TIF) techniques developed in our laboratory will be used to establish comparative biochemical profiles for structural and functional proteins isolated from rabbit and human corneas and their respective corneal equivalents. Histomorphometric data will be obtained from corneal equivalents and native rabbit and human corneas for immunoreactivity against several biomarkers of ocular irritation including: interleukin-1-alpha, fibronectin, intercellular adhesion molecule-1, heat shock protein 70 and lactate dehydrogenase. The combination of characteristic protein profiles for structural and functional proteins and the histomorphometric data for biomarkers of tissue injury will be used to establish a reference database for the corneal equivalents and the native tissues.

Corneal equivalents will be exposed to chemicals in vitro and protein biomarkers of the irritant-tissue interaction identified to alterations in the TIF and histomorphometric data when compared to the reference database. TIF and histomorphometric data will be used to: (1) rank the severity and establish a dose-response relationship for the ocular irritants, (2) explore the mechanism of selected ocular irritants and (3) directly compare the irritant response of rabbit and human organotypic models. The major goal of the proposed study is to develop the rabbit and human organotypic models as animal use alternatives in the toxicologic evaluation of compounds used by the U. S. Air Force. In addition, the use of human corneal equivalents in the in vitro exposure protocols will provide a unique basis for the extrapolation of ocular irritancy data to the potential human response.

REO  
Dr. Nicholas V. Reo

## NMR SPECTROSCOPY AS A TOOL FOR STUDIES OF HEPATOTOXICITY IN VIVO

Nuclear magnetic resonance (NMR) spectroscopy is a useful tool for studies of tissue metabolism *in vivo*, and as such, opens a new realm of exploratory possibilities in toxicology research. This methodology provides a window into the pathways of tissue biochemistry, and enables one to assess the effects of xenobiotics on endogenous metabolism and tissue function. Such studies may reveal early predictors of toxicity which is not possible through conventional toxicology testing, and can aid in our understanding of toxicological mechanisms.

This presentation will describe our research concerning the hepatotoxicity associated with perfluorocarboxylic acids, specifically perfluoro-n-octanoic acid (PFOA) and perfluoro-n-decanoic acid (PFDA). These fluorocarbons belong in a class of compounds collectively known as peroxisome proliferators (PPs). This structurally diverse group of compounds covers a range of commercial and biological utility. Unfortunately, many PPs display severe toxicity and are nongenotoxic hepatocarcinogens; the mechanisms of action are not understood.

NMR studies from our laboratory have revealed that perfluorocarboxylic acids are not metabolized, yet cause significant effects on hepatic carbohydrate and phospholipid metabolism. Following PFDA treatment in rats hepatic effects included: decreased glucose utilization, inhibition in glycogenesis, decreased utilization of glucogenic amino acids (i.e., alanine), and a significant increase in liver phosphocholine. Standard biochemical analyses have confirmed that the effect on PCho concentration is the result of an activation in liver phospholipase C. Diacylglycerol, an important second-messenger metabolite, is also significantly elevated. These results suggest that PFDA, and other PPs, may induce various metabolic effects through a mechanism involving protein kinase C activation.

Our experimental results demonstrate the utility of NMR techniques in toxicology research, and aid in our understanding of the impact of PPs on liver function. Future studies will characterize the effects of various other PPs on liver phospholipid metabolism, in an effort to delineate a common biochemical mechanism of action.

RISBY  
Dr. Terence Risby

## BIOMARKER ANALYSIS OF HUMAN BREATH FOR EARLY PREDICTION OF HEPATOTOXICITY

More than 500,000 people are occupationally exposed to tetrachloroethylene, a cleaning and degreasing solvent that is a suspected hepatotoxin. Early signs of hepatotoxicity from this agent have been difficult and expensive to detect. We propose that assessment of the risk to human health posed by realistic occupational levels of tetrachloroethylene can be made rapidly and non-invasively based on quantitative molecular epidemiology using breath biomarkers of exposure and effect.

The specific aims of this study are to: 1) identify and quantify breath sulfur-and nitrogen-containing biomarkers of liver dysfunction; 2) generate a library of these breath biomarkers for various liver diseases; 3) investigate whether increased free radical generation, as measured by levels of breath ethane, occurs as a result of a 4 hour exposure to occupational levels of tetrachloroethylene; 4) investigate whether CNS toxicity, as measured by airway occlusion pressure, occurs as a result of a 4 hour exposure to occupational levels of tetrachloroethylene; and 5) demonstrate that breath biomarkers can be used to identify people who have liver dysfunction as a result of occupational exposure to tetrachloroethylene.

ROBLEDO  
Mr. Raymond Robledo  
Dr. Mark Witten

## THE CHRONIC EFFECTS OF JP-8 JET FUEL EXPOSURE

In a simulated military flightline exposure protocol, male congenic mice and their male C57BL6 parent strain were used to investigate the pulmonary effects of aerosolized JP-8 jet fuel inhalation. The congenic mice are deficient in the induction of both aryl hydrocarbon hydroxylase (AHH) and N-acetyltransferase (NAT) enzymes. Congenic mice (MHD) were exposed nose-only daily for one hour to a  $1,036 \text{ mg/m}^3$  average of JP-8 for seven days with comparison to C57BL6 mice (BHD) similarly exposed to  $1,092 \text{ mg/m}^3$  average of JP-8 and their corresponding baseline control groups (MBC=congenic, BBC=C57BL6). JP-8 jet fuel exposure caused a significant increase in alveolar epithelial clearance to the MHD (1.22 %/min) group compared to MBC (0.44 %/min), BBC (0.38) %/min) and BHD (0.23 %/min) groups, as measured by technetium labeled diethylenetriamine pentaacetate ( $^{99\text{m}}\text{TcDTPA}$ ) clearance. Increased alveolar epithelial clearance to the MHD group was supported by a significant increase in bronchoalveolar lavage fluid (BALF) total protein ( $74.34 \text{ } \mu\text{g/ml}$ ) over MBC ( $35.83 \text{ } \mu\text{g/ml}$ ), BBC ( $34.78 \text{ } \mu\text{g/ml}$ ) and BHD ( $34.57 \text{ } \mu\text{g/ml}$ ) groups. Light microscopy showed pathological signs of alveolar edema, red blood cell infiltration, and airway inflammation for MHD as compared to all groups. The MHD group also showed a significant increase in pulmonary compliance, which was not accompanied by significant total pulmonary resistance changes with respect to its control. The pulmonary changes do not appear to be a systemic immune response, as total leukocyte counts in BALF remained unchanged. In order to determine a possible role for the neuropeptide substance P in lung injury, congenic mice were exposed similarly to  $1,000 \text{ mg/m}^3$  followed by 15 minutes of aerosolized  $1 \text{ } \mu\text{M}$  substance P (MHP) for seven days with a corresponding control group (SPC). MHP ( $0.461 \text{ %/min}$ ) had significantly lowered  $^{99\text{m}}\text{Tc-DTPA}$  clearance along with a significant decrease in BALF total protein ( $35.24 \text{ } \mu\text{g/ml}$ ), compared to control levels. Substance P also reduced pathological lung injury as determined by light microscopy. The attenuation of lung injury by substance P may be mediated through an immune response as MHP ( $2.04 \times 10^4$ ) had significantly lower total cells in BALF as compared to MHD ( $3.88 \times 10^4$ ). Supported by USAFOSR F49620-94-1-0297 and DOD AASERT Program.



HARRIS  
Dr. David T. Harris

## IMMUNOTOXICOLOGY OF EXPOSURE TO JP-8 JET FUEL AND HALOGENATED HYDROCARBONS

Inbred C57BL6 mice were exposed to either 500, 1000 or 2500 mg of aerosolized JP-8 for a period of 7 days, 1 hour of exposure per day. 24 hours after the last exposure the animals were sacrificed and the effects of exposure on the immune system examined. Immune organs (spleen, thymus, blood, lymph nodes and bone marrow) were recovered and analyzed for effects on organ weight, total cell numbers, immune cell populations (by differentials), and lymphocyte subpopulations (by flow cytometry). Assays were also performed to examine the effects of exposure on immune function. Exposure to JP-8 was found to significantly decrease the total cell numbers in spleen and thymus of the animals, even at the lowest doses utilized. Flow cytometric analyses revealed that all lymphocyte subpopulations were affected equally, although it appeared that exposure resulted in an increase in inflammatory cells. Similar effects on immune cell subpopulations were also observed in lymph nodes. In the thymus it appeared that the immature CD4+CD8+ cells were differentially lost due to exposure. In terms of immune function, JP-8 exposure resulted in a significant and profound suppression in immunological competence as assessed by mixed lymphocyte reactions to mitogens, which could not be overcome by the addition of exogenous growth factors (i.e., IL-2), at even the lowest dose of exposure. An opposite effect was observed for responses to growth factor (IL-2) alone, indicating that exposure may have initiated an inflammatory reaction. Interestingly, treatment of the exposed animals with Substance P invariably reversed the effects on all measured parameters of JP-8 exposure to almost normal levels. Thus, it appears that exposure of animals to even low doses of JP-8 has a significant suppressive effect on the immune system in terms of both immune cell numbers and immune cell function. However, it may be possible to prevent or reverse these effects by treatment of the animals with Substance P.

SIEGEL

Dr. Frank L. Siegel

Dr. Steven Kornguth

## DETOXICATION ENZYMES AS BIOMARKERS OF TOXIN EXPOSURE

Our laboratories have been investigating toxin-related changes in the expression of isoenzyme forms of the detoxication enzyme glutathione S-transferase (GST) in rodents and in human blood cells and plasma. GSTs are putative biomarkers of toxicant exposure. GST is a superfamily of about fifteen isoenzymes, each a separate gene product. GSTs are classified into four families (alpha, mu, pi and theta). The members of each family form homo- and heterodimers and share substrate specificity as well as a high degree of amino acid sequence homology. GSTs in liver are induced by carcinogens, antioxidants, dioxin, phenobarbital and other antioxidants. We have described an hplc method for quantitating the level of each GST isoenzyme in small tissue samples and methods for the sensitive cellular localization of specific GSTs by immunohistochemistry. We have mapped GST isoenzymes in brain and kidney and have found that a given cell type has a characteristic profile of GST isoenzymes. The effects of bilirubin (a neurotoxin), inorganic lead, triethyllead, JP-8 jet fuel and trichloroethane on the expression of GST isoenzymes were determined and the results indicate that GSTs are tissue biomarkers of toxin exposure. In brain, GSTs were formerly believed to be localized in non-neuronal cells; our results provide evidence for high levels of GST in cerebellar Purkinje cell neurons. In the Gunn rats, a mutant which has high levels of bilirubin due to a genetic defect, massive cell loss is seen in the central portion of cerebellum (vermis) while lateral lobes of the cerebellum are spared. In these non-vulnerable brain regions, bilirubin caused large increases in specific GSTs; these GST effects were not seen in the vermis, suggesting that GST induction is a protective adaptation. Acute and chronic exposure to inorganic lead, a toxin with primary effects on kidney, caused increases in specific GST isoenzymes; these GST increases preceded irreversible pathobiological changes in renal structure and function. Lead-related increases in kidney GST expression were dramatically exacerbated by modest reduction of dietary calcium. Dose response the time course studies of the effects of a single i.p. injection of triethyllead on GSTs in kidney, liver and whole brain and retina have been completed. Biochemical, immunohistochemical, electron microscopic and light microscopic analyses of kidney from triethyllead-treated rats are nearing completion. A single acute exposure to triethyllead caused dramatic changes in behavior; animals became very aggressive toward one another. Most kidney GST isoenzymes increased after a single i.p. injection of triethyllead (10 mg/kg). Triethyllead caused increases in specific GST isoenzymes at much lower doses than were required of inorganic lead. The pathobiological effects of organic lead in kidney differ from those previously seen with inorganic lead. The decline in specific liver GSTs is a novel effect; immunohistochemical studies now underway are designed to tell us if this decline represents the loss of specific cell type in liver which is enriched in the specific GST isoforms whose levels declined following triethyllead administration, GST isoenzymes were also mapped in retina and characteristic changes were shown to result from triethyllead exposure. A pilot study of GST isoforms in blood fractions from Hill Air Force personnel has been completed. This study demonstrated the feasibility of GST analyses on blood

samples transported from Hill AFB to our laboratory and analyzed 24 h after the blood samples were drawn. The GST activities in red blood cells, white blood cells and plasma were shown to be independent measures, probably reflecting unique isoenzyme distribution in these fractions. When blood plasma alpha class GST levels in 16 control Air Force personnel were compared to values from 16 Air Force personnel who were working with jet fuel, one of the exposed group had GST levels five times greater than the upper limits of the normal range, suggesting that this measure may be an effective exposure biomarker.

(Revised 5/30/95)

AFOSR

PREDICTIVE TOXICOLOGY PROGRAM REVIEW

31 May - 1 June 1995

Holiday Inn Conference Center/I-675  
Fairborn, Ohio

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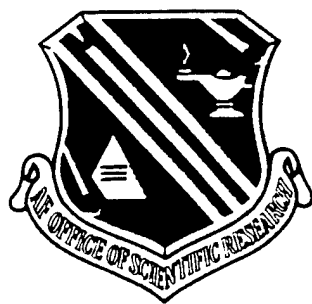
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**AIR FORCE NONLINEAR OPTICAL POLYMERS  
CONTRACTORS REVIEW MEETING**  
Holiday Inn I-675 Conference Center, Fairborn, OH  
26 February-28 February 1996

**SUNDAY, 25 FEB 1996**

3:00-7:00pm: Registration

**MONDAY, 26 FEB 1996**

7:00-8:00am: Registration/Continental Breakfast

**INTRODUCTION**

8:00-8:30am: FUTURE DIRECTIONS OF AFOSR NLO POLYMER PROGRAM  
Charles Lee, AFOSR, Chair

8:30-9:00am: GUIDED-WAVE E-O DEVICES: WHERE IS THE ACTIVE MATERIAL?  
F. Kenneth Hopkins, WL/MLPO

9:00-9:30am: COCKPIT APPLICATIONS  
Darrel Hopper, WL/AAA

9:30-9:50am: FREQUENCY CONVERSION PHENOMENA WITH POLED POLYMERS  
George Stegeman, University of Central Florida

9:50-10:10am: **BREAK**

F. Kenneth Hopkins, WL/MLPO, Chair

10:10-10:30am: FABRICATION AND LOSS MEASUREMENTS OF ETCHED  
POLYMER EO WAVEGUIDE DEVICES  
William Steier, University of Southern California

10:30-11:00am: NONLINEAR DISPERSION AND FEMTOSECOND EXPERIMENTS IN  
EPITAXIALLY GROWN PHYTHALOCYANINES AND OTHER ORGANICS  
Nasser Peyghambarian, University of Arizona

11:00-11:30am: ELECTRO-OPTIC POLYMER DEVELOPMENT  
Susan Ermer, Lockheed Martin Research and Development

11:30-12:00am: ELECTRONIC OSCILLATOR APPROACH TO OPTICAL  
NONLINEARITIES IN CONJUGATED POLYMERS  
Shaul Mukamel, University of Rochester

12:00-1:00pm:

**LUNCH**

Raymond Boncek, RL/OCPA, Chair

1:00-1:30pm: **CURRENT AF EFFORTS IN PHOTONICALLY IMPLEMENTED RF  
PHASED ARRAYS: THEORY AND PRACTICE**  
Norman P. Bernstein, RL/OCPC

1:30-2:00pm: **ELECTRO-OPTIC POLYMER DEVELOPMENT II - SUMMARY**  
Robert Gulotty, The Dow Chemical Company

2:00-2:30pm: **BIPOLARONIC CHARGE STATE INCORPORATION IN NONLINEAR  
OPTICAL MATERIALS AND POLYMERS**  
Charles W. Spangler, Northern Illinois University

2:30-3:00pm: **A SYSTEMATIC APPROACH TO ENHANCE THE THIRD ORDER  
POLARIZABILITY OF SQUARINE DYES**  
Carl Dirk, University of Texas

3:00-3:20pm: **BREAK**

Tom Cooper, WL/MLPJ, Chair

3:20-3:50pm **OPTOELECTRONIC DEVICES**  
James Grote, WL/AA

3:50-4:20pm: **OPTICAL INTERCONNECTS RELATED TO BOARD LEVEL OR  
LOCAL LEVEL COMMUNICATIONS**  
Ray Boncek, RL/OCP

4:20-4:50pm: **HIGH PERFORMANCE POLYMERS FOR ELECTRO-OPTIC  
APPLICATIONS**  
Alex Jen, ROI Technology.

4:50-5:20pm: **CURRENT PROGRESS IN  $X^{(3)}$  STUDIES**  
Anthony F. Garito, University of Pennsylvania

5:20-5:40pm: **CURRENT PROGRESS IN  $X^{(2)}$  STUDIES**  
Anthony F. Garito, University of Pennsylvania

5:40-6:00pm: **THIRD ORDER NLO RESPONSE OF DIFFUSE CHEMICAL SYSTEMS**  
Douglas S. Dudis, WL/MLBP

6:30-8:30pm: **Evening Social at Holiday Inn**



**TUESDAY, 27 FEBRUARY 1996**

**7:15-8:00am: CONTINENTAL BREAKFAST**

**Stephen Caracci, WL/MLPO, Chair**

**8:00-8:30am: RECENT ADVANCES IN THE DESIGN OF NLO MATERIALS**  
**Seth R. Marder, California Institute of Technology**

**8:30-9:00am: NEW APPROACHES TO GROWTH OF HIGHLY OPTICALLY**  
**NONLINEAR ORGANIC THIN FILMS**  
**Stephen R. Forrest, Princeton University**

**9:00-9:30am: PROGRESS TOWARD POLYMER OPTOELECTRONICS APPLICATIONS**  
**Alan J. Heeger, University of California**

**9:30-9:50am: PROGRESS TOWARDS DEVELOPING A LOW LOSS ELECTRO-OPTIC**  
**POLYMER IN THE NEAR IR**  
**William K. Bischel, Deacon Research**

**9:50-10:10am: BREAK**

**R. J. Spry, WL/MLBP, Chair**

**10:10-10:30am: ELECTRIC FIELD EFFECTS IN POLYMERS FOR SECOND**  
**ORDER NLO**  
**Hilary L. Lackritz, Purdue University**

**10:30-11:00am: DESIGN, SYNTHESIS, AND PERFORMANCE OF ADVANCED**  
**NLO-ACTIVE MOLECULAR ASSEMBLIES**  
**Tobin J. Marks, Northwestern University**

**11:00-11:30am: MECHANISMS OF THIRD ORDER OPTICAL NONLINEARITY IN**  
**QUASI-ONE AND TWO DIMENSIONAL ORGANIC SYSTEMS**  
**Sumit Mazumdar, University of Arizona**

**11:30-12:00am: THE NEEDS OF ANALOG & DIGITAL NETWORKS IN FUTURE**  
**AVIONICS ARCHITECTURES**  
**Joseph S. Wilgus, WL/AAA-1**

**12:00-1:00pm: LUNCH**

Stephen Caracci, WL/AA, Chair

- 1:00-1:30pm: NONMECHANICAL BEAM STEERING  
Philip Douville, WL/AAWW-3
- 1:30-2:00pm: MATERIALS REQUIREMENTS FOR OPTICAL LIMITING  
APPLICATIONS  
Patrick Hood, WL/MLPO
- 2:00-2:30pm: PROGRESS IN THERMALLY AND TEMPORALLY STABLE ELECTRO-  
OPTIC POLYMERS WITH WIDE OPTICAL TRANSPARENCY  
(SECOND ORDER NLO)  
Paras N. Prasad, State University of New York
- 2:30-3:00pm: RESONANT  $X^{(2)}$  PROCESSES-TWO PHOTON LASING AND OPTICAL  
POWER LIMITING  
Paras N. Prasad, State University of New York
- 3:00-3:20pm: **BREAK**

Douglas S. Dudis, WL/MLBP, Chair

- 3:20-3:40pm: AF MATERIALS RESEARCH IN SUPPORT OF OPTICAL LIMITING  
Richard L. Sutherland, SAIC
- 3:40-4:00pm: 2ND ORDER NLO POLYMER PROCESSING AND CHARACTERIZATION  
AT WPAFB  
Stephen Caracci, WL/MLPO
- 4:00-4:30pm: ADVANCES IN PHTHALOCYANINES FOR OPTICAL LIMITING  
Joe Perry, California Institute of Technology
- 4:30-5:00pm: ADVANCES IN SYNTHESIS AND PROCESSING OF SECOND-ORDER  
NONLINEAR OPTICAL MATERIALS  
Larry R. Dalton, University of Southern California
- 5:00-5:20pm: THERMAL STABILITY OF SECOND ORDER NLO CHROMOPHORES  
Ivan J. Goldfarb, Wright State University
- 5:20-5:40pm: ETALON-BASED CHARACTERIZATION AND PROBING OF  
HIGH-SPEED ELECTRONIC CIRCUITS WITH ELECTRO-OPTIC  
POLYMERS  
Vince Dominic, University of Dayton

**WEDNESDAY, 28 FEBRUARY 1996**

7:15-8:00am: **CONTINENTAL BREAKFAST**

John Zetts, WL/MLPO, Chair

8:00-8:30am: **SPACE COMMUNICATIONS**  
Carl Gass, PL/VTRA

8:30-9:00am: **IMAGE PROCESSING**  
Charles Woods, RL/EROP

9:00-9:30am: **SYNTHESIS AND CHARACTERIZATION OF 2-PHOTON RESONANT  
THIRD-ORDER NLO MATERIALS**  
Bruce A. Reinhardt, WL/MLBP

9:30-9:50am: **SYNTHESIS OF 2ND-ORDER NLO CHROMOPHORES AND POLYMERS  
FOR EO APPLICATIONS**  
Bruce A. Reinhardt, WL/MLBP

9:50-10:10am: **BREAK**

Patrick Hood, WL/MLPO, Chair

10:00-10:30am: **THERMAL STABILITY IN ELECTRO-OPTIC POLYMERS**  
Kenneth D. Singer, Case Western University

10:30-11:00am: **FABRICATION AND TESTING HIGH SPEED ELECTRO-OPTIC  
POLYMER MODULATORS FOR FIBER-OPTIC DATA LINK  
APPLICATIONS**  
Yongqiang Shi, TACAN Corporation

11:00-11:30am: **PICOSECOND ALL-OPTICAL SWITCHING USING OFF-RESONANT  
NONLINEAR REFRACTIVE INDEX OF PTS**  
Mrinal Thakur, Auburn University

11:30-12:00am: **SPACE APPLICATIONS**  
Karl W. Koch, PL/LIDN

12:00-1:00pm: **LUNCH**

Darrell Hopper, WL/AA, Chair

1:00-1:30pm: VERY LOW LOSS INTEGRATED WAVEGUIDES OF PMMA, DBR FILTER EFFECTS AND IR TWO-PHOTON PUMPED BLUE UPCONVERSION WAVEGUIDE LASERS

Anadi Mukherjee, Laser-Matter Interaction Laboratories, Inc.

1:30-2:00pm: HIGH TEMPERATURE NLO POLYMERS

Robert Miller, IBM Almaden Research Center

2:00-2:30pm: POLYMER ELECTRO-OPTIC DEVICES AND PROCESSES

John Kenney, ROI Technology

2:30-3:00pm: MULTICOLOR LITHOGRAPHY FOR REFRACTIVE INDEX GRADIENT FABRICATION

Robert Mustacich, RVM Scientific, Inc.

3:00-3:20pm: **BREAK**

Bruce A. Reinhardt, WL/MLMP, Chair

3:20-3:40pm: LD3-NLO-POLYMER-BASED GUIDED WAVE DEVICES

Ray Chen, University of Texas

3:40-4:10pm: POLYMER-BASED GUIDED-WAVE WAVELENGTH DIVISION MULTIPLEXER FOR NETWORK APPLICATIONS

Ray Chen, University of Texas

4:10-4:40pm: IMPROVING THE SYNTHESIS OF NLO CHROMOPHORES AND POLYMERIC MATERIALS

William Feld, Wright State University

4:40-5:10pm: PROGRESS IN ELECTROOPTIC POLYMERS AND COMPOSITES

Ryszard Burzynski, Laser Photonics Technology

5:10-5:20pm: **CLOSING REMARKS**

Stephen Caracci, WL/AA, Chair

- 1:00-1:30pm: NONMECHANICAL BEAM STEERING  
Philip Douville, WL/AAWW-3
- 1:30-2:00pm: MATERIALS REQUIREMENTS FOR OPTICAL LIMITING  
APPLICATIONS  
Patrick Hood, WL/MLPO
- 2:00-2:30pm: PROGRESS IN THERMALLY AND TEMPORALLY STABLE ELECTRO-  
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- 2:30-3:00p.m: RESONANT X<sup>(3)</sup> PROCESSES-TWO PHOTON LASING AND OPTICAL  
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POLYMERS  
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**WEDNESDAY, 28 FEBRUARY 1996**

**7:15-8:00am: CONTINENTAL BREAKFAST**

**John Zetts, WL/MLPO, Chair**

**8:00-8:30am: SPACE COMMUNICATIONS**  
**Carl Gass, PL/VTRA**

**8:30-9:00am: IMAGE PROCESSING**  
**Charles Woods, RL/EROP**

**9:00-9:30am: SYNTHESIS AND CHARACTERIZATION OF 2-PHOTON RESONANT**  
**THIRD-ORDER NLO MATERIALS**  
**Bruce A. Reinhardt, WL/MLBP**

**9:30-9:50am: SYNTHESIS OF 2ND-ORDER NLO CHROMOPHORES AND POLYMERS**  
**FOR EO APPLICATIONS**  
**Bruce A. Reinhardt, WL/MLBP**

**9:50-10:10am: BREAK**

**Patrick Hood, WL/MLPO, Chair**

**10:00-10:30am: THERMAL STABILITY IN ELECTRO-OPTIC POLYMERS**  
**Kenneth D. Singer, Case Western University**

**10:30-11:00am: FABRICATION AND TESTING HIGH SPEED ELECTRO-OPTIC**  
**POLYMER MODULATORS FOR FIBER-OPTIC DATA LINK**  
**APPLICATIONS**  
**Yongqiang Shi, TACAN Corporation**

**11:00-11:30am: PICOSECOND ALL-OPTICAL SWITCHING USING OFF-RESONANT**  
**NONLINEAR REFRACTIVE INDEX OF PTS**  
**Mrinal Thakur, Auburn University**

**11:30-12:00am: SPACE APPLICATIONS**  
**Karl W. Koch, PL/LIDN**

**12:00-1:00pm: LUNCH**

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**Karl W. Koch, PL/LIDN**

**12:00-1:00pm: LUNCH**

Darrell Hopper, WL/AA, Chair

1:00-1:30pm: VERY LOW LOSS INTEGRATED WAVEGUIDES OF PMMA, DBR FILTER EFFECTS AND IR TWO-PHOTON PUMPED BLUE UPCONVERSION WAVEGUIDE LASERS

Anadi Mukherjee, Laser-Matter Interaction Laboratories, Inc.

1:30-2:00pm: HIGH TEMPERATURE NLO POLYMERS

Robert Miller, IBM Almaden Research Center

2:00-2:30pm: POLYMER ELECTRO-OPTIC DEVICES AND PROCESSES

John Kenney, ROI Technology

2:30-3:00pm: MULTICOLOR LITHOGRAPHY FOR REFRACTIVE INDEX GRADIENT FABRICATION

Robert Mustacich, RVM Scientific, Inc.

3:00-3:20pm: **BREAK**

Bruce A. Reinhardt, WL/MLMP, Chair

3:20-3:40pm: LD3-NLO-POLYMER-BASED GUIDED WAVE DEVICES

Ray Chen, University of Texas

3:40-4:10pm: POLYMER-BASED GUIDED-WAVE WAVELENGTH DIVISION MULTIPLEXER FOR NETWORK APPLICATIONS

Ray Chen, University of Texas

4:10-4:40pm: IMPROVING THE SYNTHESIS OF NLO CHROMOPHORES AND POLYMERIC MATERIALS

William Feld, Wright State University

4:40-5:10pm: PROGRESS IN ELECTROOPTIC POLYMERS AND COMPOSITES

Ryszard Burzynski, Laser Photonics Technology

5:10-5:20pm: **CLOSING REMARKS**



Darrell Hopper, WL/AA, Chair

1:00-1:30pm: VERY LOW LOSS INTEGRATED WAVEGUIDES OF PMMA, DBR FILTER EFFECTS AND IR TWO-PHOTON PUMPED BLUE UPCONVERSION WAVEGUIDE LASERS

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2:30-3:00pm: MULTICOLOR LITHOGRAPHY FOR REFRACTIVE INDEX GRADIENT FABRICATION

Robert Mustacich, RVM Scientific, Inc.

3:00-3:20pm: **BREAK**

Bruce A. Reinhardt, WL/MLMP, Chair

3:20-3:40pm: LD3-NLO-POLYMER-BASED GUIDED WAVE DEVICES

Ray Chen, University of Texas

3:40-4:10pm: POLYMER-BASED GUIDED-WAVE WAVELENGTH DIVISION MULTIPLEXER FOR NETWORK APPLICATIONS

Ray Chen, University of Texas

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4:40-5:10pm: PROGRESS IN ELECTROOPTIC POLYMERS AND COMPOSITES

Ryszard Burzynski, Laser Photonics Technology

5:10-5:20pm: **CLOSING REMARKS**

## APPENDIX K

# **ANNUAL REPORT**

## **CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM**

**CONTRACT NO. F49620-95-C-0026**

**Period of Performance: 3/1/96 - 2/28/97**

**Prepared For:**

**AIR FORCE OFFICE OF SCIENTIFIC RESEARCH  
CHEMISTRY AND LIFE SCIENCES DIRECTORATE**

**Dr. Genevieve Haddad, Program Manager**

**Presented By:**

**UES, Inc.  
4401 Dayton-Xenia Road  
Dayton, OH 45432-1894**

## **INTRODUCTION**

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The first option year included: 103 Proposals that were reviewed; 3 Program/Contractor Reviews; 2 Workshops and 4 Panel Meetings.

### **A. Evaluations of Individual Research Proposals**

UES sent out 103 proposals to 373 evaluators during the performance period of 1 March 1996 through 28 February 1997.

UES has been providing the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

### **B. Contractor/Program Reviews**

A total of 3 program reviews were held during this contract year.

1. The first program review was joint and **entitled Molecular Dynamics (MD) and High Energy Density Matter (HEDM)**. It was held 2-7 June 1996 at the University of Colorado in Boulder, CO. Of the 120 attendees, 52 were speakers. The HEDM Program is designed to search for new energetic forms of matter with possible future applications to Air Force propulsion and energy storage systems. Recent advances

and accomplishments of the program were outlined at this meeting. In addition, a workshop was held on the interactions between theory and syntheses. UES acquired the meeting site and made all arrangements for the meeting including meals and audio visual equipment. UES also provided on site support.

*Dr. Michael Berman, Program Manager*

2. The second program review was in the area of **Toxicology** and was held 12-13 December 1996 at the Holiday Inn I-675 in Fairborn, OH. The purpose of this meeting was to review basic research in toxicology which is supported by or of interest to the AFOSR program in Toxicology. Each participant presented a 25 minute presentation discussing the primary objectives, results and conclusions of past research, emphasizing major accomplishments, and indicating new directions and areas of future research. The review strived to achieve several goals: to inform each participant of other work being conducted under the AFOSR Toxicology Program; to exchange scientific information; to foster collaboration; and to generate new ideas. In addition, AFOSR acquired information to facilitate technology transfers, Air Force justification of research efforts, and decision-making with respect to programmatic organization. Of the 19 in attendance, 16 were speakers. UES acquired the meeting site; made all arrangements for the meeting including meals and audio visual equipment.

*Dr. Walter Kozumbo, Program Manager*

3. The third program review entitled **New World Vista Coordination Meeting** was held 25 February 1997 at the Holiday Inn in Pasadena, CA. The purpose of the coordination meeting was to review the polymer related approved in-house tasks in the New World Vista. Topics included Global Mobility Composites, Light Weight Structural Materials for Space, Deployable Antenna Membranes, Uninhibited Aerial Vehicles and Light Weight Antenna Structures. There were eleven in attendance. UES acquired the meeting site; made all arrangements for the meeting including breaks and audio visual equipment.

*Dr. Charles Lee, Program Manager*

### **C. Workshops**

Two workshops were held during this year's effort.

1. A **DALM (Diazolumin melanin) Workshop** was held on 3-5 March 1996 at the North Redington Beach Hilton Hotel in North Redington Beach, Florida. There were 27 in attendance of which 15 were speakers. The purpose of this meeting was to review the research that has been conducted in relationship to a recently discovered slow-luminescent compound called diazolumin melanin (DALM). Since its discovery, this compound has demonstrated rather unique properties, some of which have already been exploited to produce applications related to the fields of medicine, radiation, dosimetry, and hazardous waste remediation. Another potential application for DALM is in the area of infrared sensor development. This application was addressed and included some of the planned research on infrared sensors in biological systems. Unless we acquire a

fundamental understanding of DALM, its structure and synthesis as well as its physical, chemical and biological properties, further applications-oriented progress will be slowed. Our purpose was to review what is known about the chemistry, physics and biology of DALM and its potential applications so that we may be in a better position to make good decisions concerning future basic research endeavors in this area. UES provided travel, per diem and honorarium for six advisors; acquired the meeting site; made all arrangements for the meeting including meals and audio visual equipment. In addition UES provided on site support.

*Dr. Walter Kozumbo, Program Manager*

2. A workshop on **DOD Chemistry** was held 18-20 September 1996 at the Fort Magruder Inn and Conference Center, Williamsburg, VA. UES acquired the meeting site and made arrangements for the meeting including audio visual equipment.

*Dr. Michael Berman, Program Manager*

#### **D. Panel Meetings**

Four panel meetings were held during this year's effort.

1. A panel meeting was held on **Organic Thin Film for Optical Applications** at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 9 April 1996. UES provided travel and per diem for 3 advisors in attendance as well as the meeting location and refreshments.

*Dr. Charles Lee, Program Manager*

2. A panel meeting was held on **Molecular Dynamics and Theoretical Chemistry** at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 2 May 1996. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from six outside reviewers.

*Dr. Michael Berman, Program Manager*

3. A panel meeting was held on **High Energy Density Matter** in conjunction with the Program Review on 8 June 1996 at the University of Colorado. UES made arrangements for the meeting location as well as provided travel, per diem and honorarium for three panel members. Outside reviews were secured from six reviewers.

*Dr. Michael Berman, Program Manager*

4. A second **Molecular Dynamics and Theoretical Chemistry** panel meeting was held at the Courtyard by Marriott O'Hare in Des Plaines, IL on 3 October 1996. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from sixteen outside reviewers.

*Dr. Michael Berman, Program Manager*

## **E. Advisors**

In addition to advisors provided for Program Reviews, Workshops and Panel Meetings, UES provided travel, per diem and in many cases, honorarium for the following advisors:

David H. Cohen, **Neuroscience for the DOD Evaluation of Basic Research Programs Meeting**, Institute for Defense Analysis, Arlington, VA, 22-26 April 1996

James Todd, **Visual Perception of 3-D**, Air Force Armstrong Laboratory, WPAFB, OH, 4-6 June 1996.

Michael Tarr, **Representations of Shape in Object Recognition**, Air Force Armstrong Laboratory, WPAFB, OH, 4-6 June 1996.

Charles Czeisler, **PRET Meeting**, Sam Technologies, San Francisco, CA, 31 July 1996 and Boeing Commercial Aviation, Seattle, WA, 1 August 1996.

Subhash Basak, **Computational Toxicology to evaluate and advise the AFOSR Predictive Toxicology Program in the area of mathematical modeling**, WPAFB, OH, 5-7 August 1996.

Irving Biederman, **Human Pattern Recognition**, Air Force Phillips Laboratory, Kirtland AFB, NM, 19 October 1996.

Joseph Goldberg and Stephen Hess, **Cognitive Workload**, Air Force Armstrong Laboratory, Brooks AFB, TX and WPAFB, OH, 31 October and 1 November 1996.

Marcel Adam Just and Javier Lerch, **Integrated Assessment of Workload in Decision-Making**, Air Force Armstrong Laboratory, Brooks AFB, TX and WPAFB, OH, 18 November 1996.

Bob Pozos, Deborah a. Boehm-Davis, Wayne Gray and Len Adelman, **Understanding and Measuring Cognitive Workload**, Air Force Armstrong Laboratory, Brooks AFB, TX and WPAFB, OH, 20-26 November 1996.

Gavriel Salvendy and Robert W. Proctor, **Measurement of Cognitive Workload**, Air Force Armstrong Laboratory, WPAFB, OH, December 1996.

Bellina Veronesi and Susan Leeman, **JP-8 Jet Fuel Toxicity**, University of Arizona, Tucson, AZ, 13-14 February 1997.

## **SUMMARY**

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Julien M. Christensen, Program Manager, Judith M. Flory, Program Administrator, Betty Kerans, Program Assistant, and Donna Tinley, Assistant Program Administrator. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.



## LIST OF APPENDICES

Breakdown of Research Proposals by Program Manager

Program for **Molecular Dynamics Contractor's Meeting**, University of Colorado, Boulder, Colorado, 2-5 June 1996

Program for **High Energy Density Matter Contractor's Meeting**, University of Colorado, Boulder, Colorado, 5-7 June 1996

Program for **Toxicology Program Review**, Holiday Inn Conference Center, Fairborn, Ohio, 12-13 December 1996

Program for **New World Vista Meeting**, Pasadena Holiday Inn, Pasadena, California, 25 February 1997

Program for **Workshop on DALM (Diazoluminomelanin)**, North Redington Beach Hilton Resort, North Redington Beach, Florida, 3-5 March 1996

Summary of Reviews, **Molecular Dynamics and Theoretical Chemistry Panel Meeting**, Hyatt Regency O'Hare Hotel, Rosemont, Illinois, 2 May 1996

Summary of Reviews, **High Energy Density Matter Panel Meeting**, University of Colorado, Boulder, Colorado, 8 June 1996

Summary of Reviews, **Molecular Dynamics and Theoretical Chemistry Panel Meeting**, Courtyard by Marriott O'Hare, Des Plaines, Illinois, 3 October 1996

## **BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER**

<u>PROGRAM MANAGER</u>	<u>NO. OF PROPOSALS</u>
Haddad	10
Tangney	20
Lee	25
Kozumbo	14
Kroll	1
De Long	4
Hedberg	1
Berman	22
Roach	6

**1996 Molecular Dynamics Contractors Meeting**  
**University of Colorado, Boulder, Colorado**  
**2-5 June 1996**

**Sunday, 2 June 1996**

- 6:00 - 7:00            Registration
- 7:00 - 9:30            Poster Session, Reception

**Monday, 3 June 1996**

- 8:15 - 8:30            Introductory Remarks, *Dr. Michael Berman, AFOSR*
- 8:30 - 9:00            Time Resolved Dynamics In Molecular Cluster Ions  
*Dr. W. Carl Lineberger, University of Colorado*
- 9:00 - 9:30            Stimulated Raman Pumping and Electron Detachment Dynamics  
of Carbon Cluster Anions  
*Dr. Daniel M. Neumark, University of California*
- 9:30 - 10:00           The Effective Fragment Method for Solvation  
*Dr. Mark S. Gordon, Iowa State University*
- 10:00 - 10:30           *Break*
- 10:30 - 11:00           Chemistry in the Spacecraft Environment  
*Dr. Rainer A. Dressler, Phillips Laboratory*
- 11:00 - 11:30           Potential Energy Surfaces for Some Gas Phase Reactions  
*Dr. Keiji Morokuma, Emory University*
- 11:30 - 12:00           Does Air Burn? or The Dynamics of Chemical Reactions Under  
Extreme Conditions  
*Dr. Raphael D. Levine, The Hebrew University of Jerusalem*
- 12:00 - 1:30           *Lunch*
- 1:30 - 2:00            Conformations of Macromolecules in the Gas Phase  
*Dr. Michael T. Bowers, University of California*

**Monday, 3 June 1996 (cont'd)**

- |             |  |
|-------------|--|
| 2:00 - 2:30 | Ion Rotational Distributions at Near-Threshold Photoelectron Energies<br><i>Dr. Vincent McKoy, California Institute of Technology</i>  |
| 2:30 - 3:00 | Reactive Scattering of Hyperthermal, State-Selected Molecular Ions on Surfaces<br><i>Dr. Dennis C. Jacobs, University of Notre Dame</i>                                      |
| 3:00 - 3:30 | <i>Break</i>   |
| 3:30 - 4:00 | Reactive Processes in Molecule-Surface Collisions<br><i>Dr. Curt Wittig, University of Southern California</i>   |
| 4:00 - 4:30 | Kinetic Simulations of Island Formation During Epitaxial Deposition<br><i>Prof Horia Metiu, University of California</i>   |
| 4:30 - 5:00 | Dynamics of Fracture in Nanophase Silicon Nitride: Million Atom Molecular-Dynamics Simulations on Parallel Machines<br><i>Dr. Rajiv K. Kalia, Louisiana State University</i> |

**Tuesday, 4 June 1996**

- 8:30 - 9:00            Recent Progress in Studies of Femtosecond Dynamics and Control  
of Reactions  
*Dr. Ahmed Zewail, California Institute of Technology*
- 9:00 - 9:30            Fluctuations and Relative Stability in Systems  
Far From Equilibrium  
*Dr. John Ross, Stanford University*
- 9:30 - 10:00          Vibrational Dynamics of Polyatomic Molecules in Polyatomic  
Supercritical Fluids and Liquids  
*Dr. Michael D. Fayer, Stanford University*
- 10:00 - 10:30         *Break*
- 10:30 - 11:00         Thermal Energy Reactions of Mass Selected Cluster Ions  
*Dr. Al A. Viggiano*
- 11:00 - 11:30         State Resolved Dynamics of Ion-Molecule Processes  
*Dr. Stephen R. Leone, University of Colorado*
- 11:30 - 11:45         *Break*
- 11:45 - 12:00         *Dr. Michael Berman, AFOSR*
- 12:00 - 2:00          *Lunch*
- 2:00 -                 Informal Discussions
- 7:30 - 8:00            Met-Cars: Optical Excitation and Dynamics of Ionization  
*Dr. A. Welford Castleman, Jr., The Pennsylvania State University*
- 8:00 - 8:30            Photodissociation and Photoionization of Metal Compound  
Clusters  
*Dr. Michael A. Duncan, University of Georgia*
- 8:30 - 9:00            Density Functional Theory for Large Molecules and Application to  
Metcars  
*Dr. Gustavo E. Scuseria*

**Wednesday, 5 June 1996**

- 8:30 - 9:00            Dynamics of Rotational and Vibrational non-Equilibrium in  
Thermospheric Species  
*Dr. William A. M. Blumberg, Phillips Laboratory*
- 9:00 - 9:30            Inelastic and Reactive Collision Dynamics of Atmospheric Species  
via High Resolution IR Lasers  
*Dr. David J. Nesbitt, University of Colorado*
- 9:30 - 10:00           Time- and State-Resolved Dynamics of O-Atom Reactions  
*Dr. Michael Casassa, National Institute of Standards and  
Technology*
- 10:00 - 10:30           The Collisional Coupling of the Highly Excited  $a^1\Sigma_u^-$ ,  $a^1\Pi_g$ , and  
 $w^1\Delta_u$  Electronic States of Nitrogen  
*Dr. Daniel H. Katayama, Phillips Laboratory*
- 10:30 - 11:00           *Break*
- 11:00 - 11:30           HCP $\leftrightarrow$ HPC Isomerization, Spectral Unzipping, and Triplet States  
of Acetylene  
*Dr. Robert W. Field, Massachusetts Institute of Technology*
- 11:30 - 12:00           Internal Energy in Reaction Dynamics  
*Dr. F. Fleming Crim, University of Wisconsin - Madison*
- 12:00 - 12:30           PUMP-DUMP-PROBE in Crossed and Uncrossed Molecular  
Beams  
*Dr. Alec M. Wodtke, University of Southern California, Santa  
Barbara*
- 12:30 - 1:00            Is Density Functional Theory Appropriate for Inorganic Molecular  
Anions?  
*Dr. Henry F. Schaefer, III*
- Afternoon              BBQ at Flagstaff Mt. (Joint with HEDM Meeting)

**1996 High Energy Density Matter Contractors Meeting**  
**University of Colorado, Boulder, Colorado**  
**5-7 June 1996**

**Wednesday, 5 June 1996**

Afternoon	BBQ at Flagstaff Mt. (Joint with Molecular Dynamics)
6:00 - 7:00	Registration
7:00 - 9:30	HEDM Poster Session

**Thursday, 6 June 1996**

8:30 - 8:45	Introductory Remarks, <i>Dr. Michael Berman, AFOSR</i>
8:45 - 9:00	Phillips Laboratory Remarks <i>Dr. Pat Carrick, Phillips Laboratory</i>
9:00 - 9:15	Phillips Laboratory Remarks <i>Dr. Stephen L. Rodgers, Phillips Laboratory</i>
9:15 - 9:30	<i>Break</i>
9:30 - 10:00	Solid Hydrogens Doped with Atomic and Molecular Oxygen <i>Dr. V. Ara Apkarian, University of California</i>
10:00 - 10:30	Mass Spectrometry Studies of Pick Up by Helium Clusters <i>Dr. Ken Janda, University of California</i>
10:30 - 11:00	Calorimetric Measurements of O Atom Concentration in a Solid Ar Matrix <i>Dr. Peter Taborek, University of California, Irvine</i>
11:00 - 11:30	Status Report of Cryogenic Solid Hybrid Rocket Engine Development for HEDM Demonstrations <i>Dr. Eric Rice, Orbitec, Inc.</i>
11:30 - 12:45	<i>Lunch</i>
12:45 - 1:15	Progress Towards Depositions of Velocity Selected Aluminum Atoms into Cryogenic para-Hydrogen Matrices <i>Dr. Mario E. Fajardo, Phillips Laboratory</i>

**Thursday, 6 June 1996 (cont'd)**

- 1:15 - 1:45            Spectral Theory of Physical and Chemical Binding in HEDM Systems  
*Dr. Jeffrey A. Sheehy, Phillips Laboratory*
- 1:45 - 2:15            Quantum Molecular Dynamics Simulations of Low Temperature Hydrogen Systems  
*Dr. Gregory A. Voth, University of Pennsylvania*
- 2:15 - 2:45            The Interaction of Alkali Atoms with Large Clusters of n-H<sub>2</sub>, p-H<sub>2</sub> and p-D<sub>2</sub> Probed by Laser Spectroscopy  
*Dr. Giacinto Scoles, Princeton University*
- 2:45 - 3:00            *Break*
- 3:00 - 3:30            Resonant Photoionization Spectroscopy of Al(Ar)<sub>n</sub> Clusters  
*Dr. Mitchio Okumura, California Institute of Technology*
- 3:30 - 4:00            Spectroscopic Characterization of Non-Bonding Interactions of the Boron Atom  
*Dr. Paul J. Dagdigan, The Johns Hopkins University*
- 4:00 - 4:30            Structure and Energetics of B(Ar)<sub>n</sub> and B(N<sub>2</sub>) Clusters  
*Dr. Millard H. Alexander, University of Maryland*
- 7:30                    Theory/Synthesis Workshop

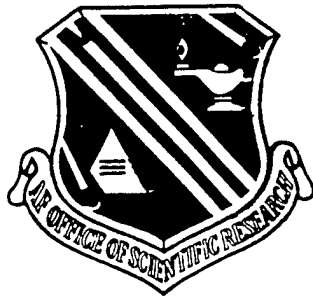


**Friday, 7 June 1996**

- |               |   |
|---------------|---|
| 8:15 - 8:45   | Cryogenic Solid Combustion<br><i>Dr. William Larson, Phillips Laboratory</i>  |
| 8:45 - 9:15   | Generation of Energetic Species in Solid Oxygen with Tunable Ultraviolet Light<br><i>Dr. Richard A. Copeland, SRI International</i>   |
| 9:15 - 9:45   | The Overtone $Q_v(0)$ Transitions in Hydrogen<br><i>Dr. Takeshi Oka, The University of Chicago</i>  |
| 9:45 - 10:15  | Search for Metallic Hydrogen in the Extended Infrared<br><i>Dr. Isaac F. Silvera, Harvard University</i>  |
| 10:15 - 10:45 | <i>Break</i>  |
| 10:45 - 11:15 | Reactions of Laser-Ablated Boron Atoms with $\text{NH}_3$ , $\text{CH}_3\text{NH}_2$ and NO to Form Novel Boron Insertion Products<br><i>Dr. Lester Andrews, University of Virginia</i> |
| 11:15 - 11:45 | Excited States for Molecules and Clusters<br><i>Dr. Rodney J. Bartlett, University of Florida</i>   |
| 11:45 - 12:15 | Nonadiabatic Processes Affecting Detection and Preparation of Energetic Materials<br><i>Dr. David R. Yarkony, Johns Hopkins University</i>  |
| 12:15 - 12:45 | Potential Energy Surfaces and Dynamics for High Energy Species<br><i>Dr. Mark S. Gordon, Iowa State University</i>  |
| 12:45 - 2:00  | <i>Lunch</i>  |
| 2:00 - 2:30   | <i>Discussion</i>   |
| 2:30 - 3:00   | Quantum Mechanical Study of the Energetics of $\text{C}_8\text{H}_8$ Hydrocarbons<br><i>Dr. E. J. Wucherer, Phillips Laboratory</i>   |
| 3:00 - 3:30   | Synthesis of High-Energy Density Materials Based on Strained-Ring Compounds<br><i>Dr. William P. Dailey, University of Pennsylvania</i>   |
| 3:30 - 3:45   | <i>Break</i>  |

**Friday, 7 June 1996 (cont'd)**

- |             |  |
|-------------|--|
| 3:45 - 4:15 | Recent Progress in the Theory and Synthesis of Novel High Energy Density Materials<br><i>Dr. Karl O. Christe, Hughes STX and Propulsion Science Division</i> |
| 4:15 - 4:45 | Extra-High Energy Oxidizers and Fuels<br><i>Dr. Robert J. Schmitt, SRI International</i>   |
| 4:45 - 5:00 | Closing Remarks, adjournment   |



**AFOSR TOXICOLOGY PROGRAM REVIEW**  
**Holiday Inn Conference Center**  
**Fairborn, Ohio**  
**12 - 13 December 1996**

**Wednesday, 11 December 1996**

1700-1830    **REGISTRATION**  
1830-2000    Evening Reception at Holiday Inn

**Thursday, 12 December 1996**

**Introductory Comments**

0730-0830    **REGISTRATION AND CONTINENTAL BREAKFAST**  
  
0830-0845    **AFOSR'S Toxicology Program**  
                 Dr. Walt Kozumbo, AFOSR, Bolling AFB, DC

**Toxicology Program at Armstrong Laboratory/Tri-Service Toxicology**

0845-0900    **Air Force Laboratory Toxicology Programs**  
                 Dr. John M. Frazier, Armstrong Laboratory, WPAFB  
  
0900-0915    **Trichlorethylene - Metabolic Pathway Modeling**  
                 Dr. Jeff Fisher, Armstrong Laboratory, WPAFB  
  
0915-0930    **Halon Replacements**  
                 Dr. Allen Vinegar, ManTech at WPAFB  
  
0930-0945    **Dermal Penetration**  
                 Dr. James N. McDougal, Geo-Centers at WPAFB  
  
0945-1000    **Total Petroleum Hydrocarbons**  
                 Captain Wade H. Weisman, Armstrong Laboratory, WPAFB  
  
1000-1015    **COFFEE BREAK**

### **In Vivo Toxic Effects/Biomarkers**

- 1015-1045    **The Role of Substance P in a Model of Chronic Exposure to JP-8 Jet Fuel**  
Mark L. Witten, University of Arizona
- 1045-1115    **Immunotoxicology of JP-8 Jet Fuel Exposure**  
David T. Harris, University of Arizona
- 1115-1145    **Detoxication Enzymes as Biomarkers of Toxin Exposure**  
Drs. Frank L. Siegel & Steven E. Kornguth, University of Wisconsin
- 1145-1215    **NMR Studies of Liver Metabolism Following Exposure to Trichloroacetate and Other Peroxisome Proliferators**  
Dr. Nicholas V. Reo, Wright State University
- 1215-1330    **LUNCHEON at Holiday Inn**
- 1330-1400    **Biomarker Analysis of Human Breath for Early Prediction of Hepatotoxicity**  
Dr. Terence H. Risby, Johns Hopkins University
- 1400-1430    **Changes in Steroid Hormone Metabolism as Noninvasive Biomarkers of Toxicant Exposure and Effect**  
Dr. Gerald A. LeBlanc, North Carolina State University

### **Mechanistically Based Toxicology**

- 1430-1500    **Mechanisms Associated With the Toxicity of Naphthalene, Chromium and Cadmium**  
Dr. Sidney J. Stohs, Creighton University
- 1500-1515    **COFFEE BREAK**
- 1515-1530    **Perfluorinated Fatty Acids of Specific Chain Lengths Directly Inhibit Gap Junctional Intercellular Communication and Indirectly Inhibit via H<sub>2</sub>O<sub>2</sub> in Glutathione-Sufficient But Not Glutathione-Deficient Cells**  
Dr. Brad L. Upham, Michigan State University
- 1530-1600    **Chromium Toxicity: Reductive Enzymes in Humans**  
Dr. Charles R. Myers, Medical College of Wisconsin
- 1600-1630    **Depletion of Nuclear Poly (ADP-ribose) Polymerase by Antisense RNA Expression: Influences on DNA Repair and Replication, and Survival of Cells to Genotoxic Agents. New Studies on Apoptosis.**  
Dr. Mark E. Smulson, Georgetown University
- 1630-        **Discussion and adjournment until tomorrow morning.**

**Friday, 13 December 1996**

**0730-0830 CONTINENTAL BREAKFAST at Holiday Inn**

**Predictive Toxicology: Alternatives to Animal Use in Toxicity Assessment**

**0830-0900 An Interdisciplinary and Alternative Approach to Assess Carcinogenicity of Chlorobenzenes**

Dr. Raymond S.H. Yang, Colorado State University

**0900-0930 Predictive Toxicology**

Dr. John M. Frazier, Armstrong Laboratory, WPAFB

**0930-1000 Corneal Equivalents for In Vitro Testing of Ocular Irritants**

Dr. Thomas E. Eurell, University of Illinois

**1000-1015 COFFEE BREAK**

**1015-1045 Protein Biomarkers of Chemical Exposure and Molecular Toxicology**

Dr. Frank A. Witzmann, Indiana University-Purdue University  
at Indianapolis

**1045-1115 Development of QMSA and QSAR Methods for Hazard Assessment of Chemicals: Tools for Computational Toxicology**

Dr. Subhash C. Basak, University of Minnesota

**1115-1200 Open discussion and concluding remarks.**

New World Vista Meeting February 25, 1997

Pasadena Holiday Inn Hotel (Room #)

- 8:00 Breakfast  
8:30 Opening Remarks (Overview of NWV)  
9:00 Discussion Session  
9:30 Scott Wierschke (Polymers in Rocket Applications)  
1000 Break  
  
*(Low Cost, Light Weight Membrane Structure - Antenna)*  
1030 Jonathan Bishop - PL  
1100 Derrick Dean -WL  
*(Family of Unmanned Aerial Vehicle)*  
1120 Dave Curliss (WL)  
*(Air Mobility - Composites)*  
1140 Frances Abrams  
(Carbon Foams)  
1200 Lunch  
  
*(Light Weight Structure and Materials in Space)*  
1300 Steve Rogers/ Wade Adams (PL/ML)  
1310 Kevin Chaffee - PL  
Polymer Innovation for Rocket Propulsion  
1330 Richard Vaia - (WL)  
Advanced Light Weight Materials  
1350 Charles Stein (PL)  
Synergism in the Interaction of Atomic Oxygen, Electrons, and UV  
Radiation with Organic Polymers  
1410 Wes Hoffman (PL)  
Light Weight, Low Cost Rocket Propulsion Manufacturing Technology  
1430 Alok Das (PL)  
Theoretical and Experimental Studies of Vibronacoustic Systems  
1440 Break  
  
1500 Closed Session (Government Only)



**AFOSR Workshop on DALM (Diazoluminomelanin)**  
**North Redington Beach Hilton Resort, North Redington Beach, FL**  
**3-5 March 1996**

**Sunday, 3 March 1996**

- 1700-1830    **REGISTRATION** (The Verandah adjacent to hotel restaurant)  
1830-2030    **Evening Reception** at North Redington Beach Hilton Resort  
                  (The Verandah)

**Monday, 4 March 1996**

**Introduction**

- 0730-0800    **REGISTRATION AND CONTINENTAL BREAKFAST**  
                  (Conference Rooms C & D)
- 0800-0810    **Welcome and Meeting Objectives**  
                  Dr. Walt Kozumbo, AFOSR, Bolling AFB, DC
- 0810-0830    **Historical Perspective and Potential Importance of DALM**  
                  Dr. Johnathan Kiel, Armstrong Lab., Brooks AFB, TX

**Properties, Structure and Synthesis of DALM (Dr. Kiel as Moderator)**

- 0830-0900    **Organic Synthesis of DALM**  
                  Mr. Gerald O'Brien, SAIC, San Antonio, TX
- 0900-0930    **Instrumentation for Real Time Measurement of DALM Luminescence**  
                  Mr. Brion Burghard, Pacific Northwest National Labs., Richland, WA
- 0930-1000    **Chemical Structure of DALM Based on NMR**  
                  Dr. John Wright, Southeastern Oklahoma State Univ., Durant, OK
- 1000-1015    **COFFEE BREAK**
- 1015-1045    **Biosynthesis of DALM**  
                  TSgt. John L. Alls, Armstrong Lab., Brooks AFB, TX
- 1045-1115    **Molecular Biology of DALM Biosynthesis**  
                  Dr. Jill E. Parker, Armstrong Lab., Brooks AFB, TX

1115-1145 Purification & Characterization of Bacillus Anthracis Aerobic Nitrate Reductase (Dalm Synthase)  
Lt. Col. Larry D. Strawser, US Air Force Academy, Colorado Springs, CO

1145-1200 Discussion

1200-1330 LUNCH (The Verandah)

1330-1400 Biosynthesis of DALM in HL-60 Cells and Other Attempts of Eukaryotic Cell Biosynthesis  
Dr. John G. Bruno, Applied Research Assoc., Tyndall AFB, FL

1400-1430 Molecular Modeling and the Discovery of the Solid State Properties of DALM  
Maj. Eric A. Holwitt, Armstrong Lab., Brooks AFB, TX

**Potential Applications of DALM (Maj. Eric A. Holwitt as Moderator)**

1430-1500 Requirement for New RFR Dosimetric Techniques Using DALM  
Dr. Johnathan L. Kiel, Armstrong Lab., Brooks AFB, TX

1500-1530 DALM and Other Poly-Monohydroxyarylamino Acids as Antibiotics  
Dr. Johnathan L. Kiel, Armstrong Lab., Brooks AFB, TX

1530-1545 COFFEE BREAK

1545-1600 Metallo-DALM Complexes as Catalysts for Hydrazine Breakdown  
Maj. Eric A. Holwitt, Armstrong Lab., Brooks AFB, TX

1600-1630 The SERDP Project: Metallo-DALM for the Remediation of Hydrazines  
Lt. David J. Kuch, Armstrong Lab., Tyndall AFB, FL

1630-1700 Discussion

1700 Adjournment until tomorrow morning

**Tuesday, 5 March 1996**

0730-0830 CONTINENTAL BREAKFAST (Conference Rooms C & D)

**Role of DALM in the AFOSR Biomimetic Infrared Sensor Initiative**

0830-0900 DALM as a Photoreactive Material and Its Use in IR Sensors  
Dr. Thomas Cooper, Wright Lab., Wright-Patterson AFB, OH  
Dr. John Taboada, Armstrong Lab., Brooks AFB, TX



- 0900-0930    **Infrared Sensing in Pit Vipers**  
                 Dr. Richard C. Goris, Yokohama City University, Yokohama, Japan
- 0930-1000    **Infrared Sensing in Boids**  
                 Dr. Michael S. Grace, University of VA., Charlottesville, VA
- 1000-1015    **COFFEE BREAK**
- 1015-1045    **Infrared Sensing in Single-Cell Organelles**  
                 Dr. Guenter Albrecht-Buehler, Northwestern Univ., Chicago, IL
- 1045-1100    **Discussion and adjournment**
- 1100-1300    **LUNCH (on your own)**  
                 Meeting of Reviewers and Program Managers at Hotel

**SUMMARY OF REVIEWS**  
**Molecular Dynamics Panel Meeting**

- 96-NL-096    Partitioning and Reactivity of Environmental Solutes in Multiphase Systems**  
- Donald G. Truhlar, University of Minnesota

Steven D. Colson, Pacific Northwest Laboratory ( )  
Jeff Hay, Los Alamos National Laboratory (A/1)  
George Schatz, Northwestern University (A-/3)  
Ann B. McCoy, Ohio State University (A/3)

- 96-NL-131    Atomic Scale Chemistry and Structure of Ceramic/Metal Interfaces**  
- David N. Seidman, Northwestern University

Steven D. Colson, Pacific Northwest Laboratories ( )  
Jeff Hay, Los Alamos National Laboratory (A-/2)  
J. Michael White, University of Texas (A-/3)  
David Vanderbilt, Rutgers University (A-/4)

- 96-NL-135    Physical Chemistry of Energetic Nitrogen Compounds**  
- Robert D. Coombe, University of Denver

Laurie J. Butler, University of Chicago (A-/B+/2/-4/5)  
Charles Parmenter, Indiana University (A-/3>4)  
James Weisshaar, University of Denver (A/4)  
J. Michael White, University of Texas (A/1)  
David Benard, Rockwell Science Center (A/1)

- 96-NL-136    Spectroscopy of Anions and Transition States Using Stimulated Raman Pumping**  
- Daniel M. Neumark, University of California

Laurie J. Butler, University of Chicago (A/A-/2)  
Charles Parmenter, Indiana University (A/3)  
George Schatz, Northwestern University (A+/1)  
James Weisshaar, University of Denver (A/1)

- 96-NL-137    **Theoretical Methods for Optimal Design of Biomaterials:  
Energy Landscape Perspective**  
Devarajan Thirumalai, University of Maryland

Jeff Hay, University of Maryland (B+/2)

George Schatz, Northwestern University (B/3)

Bruce Garrett, Pacific Northwest Laboratory (A/A-/2)

Kenneth Jordan, University of Pittsburgh (A/4)

- 96-NL-138    **Triplet States of Small Molecules: Photochemistry, Spectroscopy, and  
Dynamics**  
- Robert W. Field, Massachusetts Institute of Technology

Laurie J. Butler, University of Chicago (A/2)

Steven D. Colson, Pacific Northwest Laboratory ( )

Charles Parmenter, Indiana University (A/2)

James Weisshaar, University of Wisconsin (A+/2)

- 96-NL-140    **Clusters of Transition Metal Compounds: Building Blocks of New Materials**  
- Albert Welford Castleman, Jr., Pennsylvania State University

Laurie J. Butler, University of Chicago (A/A-/3)

Steven D. Colson, Pacific Northwest Laboratory ( )

Charles Parmenter, Indiana University (A/3)

James Weisshaar, University of Wisconsin (B+/2)

J. Michael White, University of Texas (A+/2)

- 96-NL-148    **Optimization of Geometric Structures of New Materials on Parallel  
Computers**  
- John H. Weare, University of California

Jeff Hay, Los Alamos National Laboratory (A/2)

George Schatz, Northwestern University (B+/2)

J. Michael White, University of Texas (-/4)

Albert F. Wagner, Argonne National Laboratory (A-/B+/2)

**SUMMARY OF REVIEWS**  
**High Energy Density Matter Panel Meeting**

- 96-NL-133    Reactions of Laser-Ablated Metal Atoms to Produce High Energy Molecules**  
- Lester Andrews, University of Virginia

Vladimir E. Bondybey, Technical University of Munich (A-/1)  
Bruce C. Garrett, Pacific Northwest National Laboratory (A/3)  
Clark W. Hawk, UAH Propulsion Research Center (B+/5)  
Lon B. Knight, Furman University (A+/2)  
James J. Valentini, Columbia University (A/2)  
John S. Winn, Dartmouth College (A/2)  
Derek M. Lindsay, City University of New York, City College (A/2)

- 96-NL-147    Spectroscopy of Metal Atoms Trapped in Solid Helium**  
- Ken G. Libbrecht, California Institute of Technology

Vladimir E. Bondybey, Technical University of Munich (B+/1)  
Bruce C. Garrett, Pacific Northwest National Laboratory (A-/B+/3)  
Clark W. Hawk, UAH Propulsion Research Center (A/5)  
Marilyn Jacox, National Institute of Standards & Technology (B+/1)  
Derek M. Lindsay, City University of New York, City College (B+/2)  
James J. Valentini, Columbia University (B/2)

- 96-NL-153    Spectroscopic and Dynamical Studies of Impurities in Solid Hydrogen:  
A Possible Road to HEDM**  
- Takeshi Oka, The University of Chicago

Vladimir E. Bondybey, Technical University of Munich (A+/1)  
Bruce C. Garrett, Pacific Northwest National Laboratory (A+/3)  
Clark W. Hawk, UAH Propulsion Research Center (B/5)  
Terry A. Miller, Ohio State University (A/3)  
James J. Valentini, Columbia University (A-/2)  
John S. Winn, Dartmouth College (A/1)

October 3, 1996

**SUMMARY OF REVIEWS**  
**AFOSR Molecular Dynamics/Theoretical Chemistry Review Panel**

- 96-NL-190    Femtosecond Shock Wave Dynamics of Insensitive Energetic Materials**  
- Dana D. Dlott, University of Illinois

Thomas B. Brill, University of Delaware (A/3)  
Laurie J. Butler, University of Chicago (A-/B+/4/5)  
Charles S. Parmenter, Indiana University (A/3)  
James C. Weisshaar, University of Wisconsin ((A/4)  
J. Michael White, University of Texas at Austin (A+/1)

- 96-NL-201    State-Resolved Thermal/Hyperthermal Collision Dynamics of Atmospheric Species**  
- David J. Nesbitt (University of Colorado)

Laurie J. Butler, University of Chicago (A/2)  
Paul L. Houston, Cornell University (A/1)  
Charles S. Parmenter, Indiana University (A-/2)  
James C. Weisshaar, University of Wisconsin (A+/2)

- 96-NL-202    Ultrafast Nonlinear Optical Investigations of Subcritical Fluids**  
- Michael D. Fayer, Stanford University

Joan F. Brennecke, University of Notre Dame (A-/2)  
Laurie J. Butler, University of Chicago (A-/4)  
Charles S. Parmenter, Indiana University (A-/3)  
Theodore W. Randolph, University of Colorado (A-/2)  
George Schatz, Northwestern University (A/3)  
J. Michael White, University of Texas at Austin (A/2)

- 96-NL-205    Chemistry Under Extreme Conditions**  
- James L. Kinsey, Rice University

Charles S. Parmenter, Indiana University (B+/4)  
Lawrence R. Pratt, Los Alamos National Laboratory (A/4-5)  
George Schatz, Northwestern University (A/2)  
John Tully, Yale University (A+/1)

- 96-NL-208    **A New Method for Fast and Accurate Atomic-Scale Simulation of Materials and Its Application to Thin-Film Epitaxy**  
 - Kristen Fichthorn, Pennsylvania State University
- Lawrence R. Pratt, Los Alamos National Laboratory (B/1)  
 Lionel M. Raff, Oklahoma State University (B+/2)  
 George Schatz, Northwestern University (A-/2)  
 Arthur F. Voter, Los Alamos National Laboratory (B+/A//1)  
 J. Michael White, University of Texas at Austin (B+/1)
- 96-NL-209    **Dynamics of Metal Species of Atmospheric Importance**  
 - John Lombardi, City College of City University of New York
- Steven D. Colson, Pacific Northwest National Laboratory (A-/2)  
 Michael D. Morse, University of Utah (A-/B+/2)  
 James C. Weisshaar, University of Wisconsin (C/1)  
 J. Michael White, University of Texas at Austin (B+/2)
- 96-NL-210    **Development and Applications of Quantum Molecular Solvation Theory Reactions in Solutions**  
 - Thanh N. Truong, University of Utah
- Jiali Gao, State University of New York at Buffalo (A-/1)  
 Lawrence R. Pratt, Los Alamos National Laboratory (B+/1)  
 George Schatz, Northwestern University (A-/B+/3)  
 Walter Stevens, National Inst. of Standards & Technology (B+/4)
- 96-NL-211    **Structure and Dynamics of Metal-Containing Clusters**  
 - Michael A. Duncan, University of Georgia
- Peter B. Armentrout, University of Utah (A/1)  
 Laurie J. Butler, University of Chicago (A/3)  
 Steven D. Colson, Pacific Northwest National Laboratory (A+/1)  
 James C. Weisshaar, University of Wisconsin (A-/1)
- 96-NL-213    **Theoretical Determination of Optimized Structures for Molecular Complexes and Clusters**  
 -Peter Pulay, University of Arkansas
- Frank Jensen, Odense University, Denmark (A/1)  
 Lawrence R. Pratt, Los Alamos National Laboratory (A/4-5)  
 George Schatz, Northwestern University (A-/2)  
 Michael C. Zerner, University of Florida (A+/1)

- 96-NL-214    A Fundamental Investigation of Metal/Ceramic Interfaces: Toward Nanostructure Control**  
- Randall Boehm, New Mexico Highlands University

Steven D. Colson, Pacific Northwest National Laboratory (B+/4)

David A. Dixon, Pacific Northwest National Laboratory (C/1)

Theodore E. Madey, Rutgers University (B/2)

J. Michael White, University of Texas at Austin (B-/2)

(A for the problem, C for the method)

- 96-NL-219    Pulsed Field Ionization Spectroscopy of Mesospheric Molecules: Elucidating the Chemistry of Metal Atoms in the Upper Atmosphere**  
- Mitchio Okumura, California Institute of Technology

Kit H. Bowen, Jr., Johns Hopkins University (A+/2)

Laurie J. Butler, University of Chicago (A/A-/3)

Steven D. Colson, Pacific Northwest National Laboratory (A/1)

Charles S. Parmenter, Indiana University (A-/B+/3)

James C. Weisshaar, University of Wisconsin (A-/2)

## APPENDIX L



# **ANNUAL REPORT**

## **CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM**

**CONTRACT NO. F49620-95-C-0026**

**Period of Performance: 3/1/97 - 2/28/98**

**Prepared For:**

**AIR FORCE OFFICE OF SCIENTIFIC RESEARCH  
CHEMISTRY AND LIFE SCIENCES DIRECTORATE**

**Dr. Genevieve Haddad, Program Manager**

**Presented By:**

**UES, Inc.  
4401 Dayton-Xenia Road  
Dayton, OH 45432-1894**

## **INTRODUCTION**

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology; Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The second option year included: 138 Proposals that were reviewed;  
7 Program/Contractor Reviews; 3 Workshops and 4 Panel Meetings.

### **A. Evaluations of Individual Research Proposals**

UES sent out 138 proposals to 422 evaluators during the performance period of 1 March 1997 through 28 February 1998.

UES has been providing the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

### **B. Contractor/Program Reviews**

A total of 8 program reviews were held during this contract year.

1. The first program review was in the area of **Polymer Composites** and was held in Anaheim, California on 9 May 1997 at the Hilton Hotel. There were 9 presenters. This was held in conjunction with the 42d SAMPE Symposium & Exhibition. UES provided travel for one advisor and honorarium for 4 advisors. UES provided acquisition of

meeting site including coffee breaks and continental breakfast and audio visual equipment.  
*Dr. Charles Lee, Program Manager*

2. The second program review was a joint ONR/AFOSR **Nonlinear Optical Polymer** review of research in the area of polymer science pertaining to optical applications. Two Multidisciplinary University Research Initiatives, an Accelerated Capabilities Initiative, and individual research efforts will be reviewed. The Air Force portion of the review was limited to second and third order NLO polymers and organics. Other topics such as photorefractive polymers were reviewed in a separate meeting. It was held 1-5 June 1997 at the Sea Turtle Inn, Jacksonville, Florida. Of the 43 attendees, 33 were speakers. ONR was the host; therefore, UES's role was to invite Air Force representatives and speakers.

*Dr. Charles Lee, Program Manager*

3. The third program review was entitled **High Energy Density Matter (HEDM)**. It was held 1-3 June 1997 at the Westfields International Conference Center in Chantilly, Virginia. The HEDM Program is designed to search for new energetic forms of matter with possible future applications to Air Force propulsion and energy storage systems. Recent advances and accomplishments of the program and future program direction was outlined at this meeting. There were 62 in attendance of which 32 were speakers and 13 provided posters at the poster session. UES also provided on-site support, made all arrangements for the meeting including meals and audio visual equipment. UES provided travel and per diem for 3 advisors who attended the HEDM meeting.

*Dr. Michael Berman, Program Manager*

4. The fourth program review was in the area of **Tribology** and was held 24-26 June 1997 at the Holiday Inn in Englewood, Ohio. This was a joint Air Force/Navy meeting. Of the 54 in attendance, 36 were speakers. UES also provided on-site support, acquisition of meeting site and audio visual equipment.

*Major Hugh De Long, Program Manager*

5. The **Chronobiology** program review was the fifth of the contract year. It was held 18-20 September 1997 at the Air Force Academy in Colorado Springs, Colorado. All funded research efforts in this program were reviewed. Invited Air Force laboratory scientists and relevant extramural scientists funded through the AFOSR Cognitive Sciences Program provided presentations. Of the 67 attendees, 31 gave oral presentations. UES provided travel and per diem for 10 advisors and honorarium for 7 advisors who attended the Chronobiology program review. UES also provided on-site support, made all arrangements for the meeting including meals and audio visual equipment.

*Dr. Genevieve Haddad, Program Manager*

6. The sixth program review was in the area of **Rocket Impact of Stratospheric Ozone** held at the National Academy of Sciences' Beckman Center in Irvine, California on

9 January 1998. The purpose of the meeting was to provide program progress and status of the work that has been carried out in the area of Atmospheric Effects of Rocket Exhausts. Twelve scientists assessed the progress and future direction of the program. UES provided acquisition of meeting site and audio visual equipment.

*Dr. Michael Berman, Program Manager*

7. The seventh program review was a joint Air Force/Navy review on **Electrochemistry**. It was held 15-16 January, 1998 in Ventura, California at the Doubletree Inn. The Air Force portion of the meeting focused on compact power. Of the 45 attendees, 38 were speakers. We provided travel expenses for one advisor. UES provided on site support, made all arrangements for the meeting including meals and audio visual equipment.

*Major Hugh De Long, Program Manager*

8. The final program review for this year was in the area of **Nanoscale Devices and Novel Engineered Materials**. It was held in Clearwater, Florida on 17-18 February 1998 at the Holiday Inn SunSpree Resort. UES provided on site support, made all arrangements for the meeting including meals and audio visual equipment. Eighteen people were in attendance.

*Major Hugh De Long, Program Manager*

### **C. Workshops**

Two workshops were held during this year's effort.

1. The first workshop focused on **Composite Durability**. It was held at the Dearborn Inn in Dearborn, Michigan on 9 October 1997. Of the 17 in attendance, 11 provided talks. UES provided on site support, made all arrangements for the meeting including meals and audio visual equipment.

*Dr. Charles Lee, Program Manager*

2. The second workshop was entitled **New World Vista Kickoff**, was held at the Marriott Riverwalk in San Antonio, Texas on 16 May 1997. Seventeen people were in attendance of which 11 provided talks. Some areas discussed were: Distributed Team Decision-Making and Performance in Complex Environments; Uninhabited Combat Air Vehicle (UCAV) Training Research Testbed; EEG-Based Online Cognitive Load Monitor; Integrated Cognitive, Computational and Biological Assessment of Workload in Decision Making. UES made all arrangements for the meeting including meals and audio visual equipment.

*Dr. John Tangney, Program Manager*

#### **D. Panel Meetings**

Four panel meetings were held during this year's effort.

1. A panel meeting was held on 20 May 1997 on **Durable Coatings** at WPAFB, Ohio. There were 9 presenters.

*Dr. Charles Lee, Program Manager*

2. A panel meeting was held on **Molecular Dynamics and Theoretical Chemistry** at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 22 May 1997. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from eighteen outside reviewers.

*Dr. Michael Berman, Program Manager*

3. A second **Molecular Dynamics and Theoretical Chemistry** panel meeting was held at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 6 November 1997. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from seventeen outside reviewers.

*Dr. Michael Berman, Program Manager*

4. The third panel meeting was on the subject of **STTR** and was held at the Holiday Inn Fairborn in Fairborn, Ohio on 3 February 1998. UES made arrangements for the meeting location. There were nine presentations along with Government meetings.

*Dr. Charles Lee, Program Manager*

#### **E. Advisors**

In addition to advisors provided for Program Reviews, Workshops and Panel Meetings, UES provided travel, per diem and in many cases, honorarium for the following advisors:

Steven Zucker, **Human Visual Processing**, Air Force Office of Scientific Research, Bolling AFB, D.C.; 24 April 1997.

Tom Triscari, **Team Performance Measurement**, Air Force Armstrong Laboratory, Brooks AFB, Texas, 11-12 March 1997.

V. C. Ramesh, **Team Performance Measurement**, Air Force Armstrong Laboratory, Brooks AFB, Texas, 24-25 March 1997.

Martin Zatz, **TARA Meeting**, Arlington, Virginia, 17-20 March 1997.

Stephen Boppart, **Predictive Toxicology Initiative** and present a seminar on the use of optical coherence tomography in assessing potential teratogenic effects of toxic agents, Wright-Patterson Air Force Base, Ohio, 3 June 1997.

A. V. Phelps, **Weakly Ionized Gases**, USAF Academy, Colorado Springs, Colorado, 9-13 June 1997.

Lt Col David Brown, **PRET Meeting**, San Francisco Hilton, San Francisco, California, 11 June 1997.

Charles Woods, **Photorefractive Meeting**, University of California, San Diego, California, 26 July 1997.

Joan Fuller, **5<sup>th</sup> International Conference on Molten Salts**, Dresden, Germany, 23-29 August 1997.

## **SUMMARY**

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Judith M. Flory, Program Administrative Manager, and Donna Tinley, Assistant Program Administrator. Upon their retirements, Dr. Julien M. Christensen was replaced by Dr. Thomas Eggemeier as Program Manager and Betty Kerans was replaced by Ann Corbitt as Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

## LIST OF APPENDICES

Breakdown of Research Proposals by Program Manager

Program for **Polymer Composites Program Review**, Hilton Hotel, Anaheim, California, 8 May 1997

Program for **Nonlinear Optical Polymer Program Review**, Sea Turtle Inn, Jacksonville, Florida, 1-5 June 1997

Program for **High Energy Density Matter (HEDM) Program Review**, Westfields International Conference Center, Chantilly, Virginia, 1-3 June 1997

Program for **Tribology Program Review**, Holiday Inn, Englewood, Ohio, 24-26 June 1997

Program for **Chronobiology Program Review**, Air Force Academy, Colorado Springs, Colorado, 18-20 September 1997

Program for **Electrochemistry Program Review**, Doubletree Inn, Ventura, California, 15-16 January 1998

Program for **Nanoscale Devices and Novel Engineered Materials**, Holiday Inn SunSpree Resort, Clearwater, Florida, 17-18 February 1998

Program for **Composite Durability Workshop**, Dearborn Inn, Dearborn, Michigan, 9 October 1997

Program for **New World Vista Kickoff Workshop**, Marriott Riverwalk, San Antonio, Texas, 16 May 1997

Program for **Durable Coatings**, WPAFB, Ohio, 20 May 1997

Program for **Molecular Dynamics and Theoretical Chemistry**, Hyatt Regency O'Hare Hotel, Rosemont, Illinois, 22 May 1997

Program for **Molecular Dynamics and Theoretical Chemistry**, Hyatt Regency O'Hare Hotel, Rosemont, Illinois, 6 November 1997

Program for **STTR**, Holiday Inn, Fairborn, Ohio, 3 February 1998



# **BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER**

<u>PROGRAM MANAGER</u>	<u>NO. OF PROPOSALS</u>
Haddad	12
Tangney	18
Lee	15
Kozumbo	35
Bellaire	14
De Long	11
Berman	29
Roach	4

**42nd International SAMPE Symposium and Exhibition**  
Anaheim Convention Center  
Anaheim, CA

**"Basic Research Challenges in Polymeric Composite Materials and Processing."**  
May 8, 1997, Room B2, Hall B

- |           |   |
|-----------|---|
| 1:00-1:10 | Opening Remarks<br><i>Dr. Charles Lee, AFOSR/NL</i>   |
| 1:10-1:40 | Air Force Basic Research Challenges for Structural<br>Polymers and Polymeric Matrix Composites<br><i>Dr. Charles Browning, WL MLB</i> |
| 1:40-2:10 | High Temperature Composite Systems<br><i>Dr. John Hoggatt, Boeing Company</i>   |
| 2:10-2:40 | Advanced Materials and Structures -<br>Requirements for Future Research<br><i>Mr. Cecil Schneider, Lockheed-Martin</i>                |
| 2:40-3:00 | <i>Break</i>  |
| 3:00-3:30 | High Performance Polymers and Composites:<br>Basic Issues<br><i>Dr. Norm Johnston, NASA Langley</i>                                   |
| 3:30-4:00 | Northrop Grumman's Prospective on Technology Voids in<br>Polymer Composites M & P<br><i>Mr. Robert Koon, Northrop Grumman</i>         |
| 4:00-4:30 | M & P Issues/Needs for PMCs at GE Aircraft Engines<br><i>Dr. William McCormack, GE-Evansdale</i>                                      |

# SCHEDULE FOR 1997 ONR/AFOSR POLYMER PROGRAM REVIEW

Polymers for Electro-Optic Applications  
Kenneth J. Wynne, ONR Program Manager  
Charles Y-C. Lee, AFOSR Program Manager

## Sunday, 1 June

11:30 am REGISTRATION  
12:30 pm Introductory Remarks - K. J. Wynne and C. Lee  
1:00 Univ of AZ: MURI Overview - Peyghambarian  
1:45 Grubbs  
2:15 Marks  
2:45 BREAK  
3:00 Jen  
3:30 Marder  
4:00 Kippelin  
4:30 Perry  
5:00 BREAK  
5:15 Dirk  
5:30 Ratner  
5:45 ADJOURN  
6:00 Navy Panel - Wynne, et.al.

## Monday, 2 June

7:30 am REGISTRATION & BREAKFAST  
8:00 Univ of MA MURI Review - Tripathy/Rubner  
10:30 BREAK  
10:45 USC ACI Review - Steier  
12:15 pm LUNCH

## ONR-Funded Individual Project Reviews

1:30 Novak  
2:00 Wright  
2:30 MacDiarmid  
3:00 BREAK  
3:15 Bazan  
3:45 Epstein  
4:15 ADJOURN  
4:30 Navy Panel

## Tuesday, 3 June

7:00 am BREAKFAST  
8:00 Hammond  
8:30 Natansohn  
9:00 Green  
9:30 Jenekhe  
10:00 BREAK  
10:15 Stupp  
10:45 Tour  
11:15 Asher  
11:45 LUNCH  
  
1:00 pm Yu  
1:30 Therein  
2:00 Shashidhar  
2:30 Heeger  
3:00 BREAK  
3:15 Lindsay  
3:45 Herman  
4:15 ADJOURN  
4:30 Navy Panel

**Wednesday, 4 June****AFOSR-Funded Individual Project Reviews**

7:00 am REGISTRATION & BREAKFAST  
8:00 Hopkins  
8:30 Pather  
9:00 Marder  
9:30 Dalton  
10:00 BREAK  
10:15 Heeger  
10:45 Prasad  
11:15 Forrest  
11:45 LUNCH

1:00 pm Garito  
1:30 Thakur  
2:00 Peyghambarian  
2:30 Marks  
3:00 BREAK  
3:15 Caracci  
3:45 Ermer  
4:15 Kuzyk  
4:45 Dirk  
5:15 ADJOURN

**Thursday, 5 June**

7:00 am BREAKFAST  
8:00 Dudis  
8:30 Reinhardt  
9:00 Stegeman  
9:30 Spangler  
10:00 BREAK  
10:15 Jen  
10:45 Kenney  
11:15 Steier  
11:45 LUNCH

1:00 pm Perry  
1:30 Bjorkland  
2:00 Shi  
2:30 Chen  
3:00 BREAK  
3:15 Bischel  
3:45 Mustavich  
4:15 Tang  
4:45 Burzynski  
5:15 CLOSE

**1997 High Energy Density Matter Contractor's Meeting**  
**Westfields International Conference Center**  
**Chantilly, VA**  
**1-3 June 1997**

**Sunday, 1 June 1997**

12:00 - 1:00	Registration
1:00 - 1:30	Introductory Remarks: <i>Dr. Michael R. Berman, AFOSR</i>
1:30 - 2:00	Propellant R&D for the Integrated High Pay-Off Rocket Propulsion Technology (IHRPT) Program <i>Dr. Patrick G. Carrick, Phillips Laboratory</i>
2:00 - 2:30	Solid Rocket Propellants Present and Future <i>Dr. Lou Cannizzo, Thiokol Corporation</i>
2:30 - 3:00	New Energetic Ingredients for High Performance Solid Propellants <i>Dr. Kenneth O. Hartman, Alliant Techsystems</i>
3:00 - 3:30	<i>Break</i>
3:30 - 4:00	Aspects of Solid and Liquid Propellant Development at Phillips Laboratory <i>Dr. Tom W. Hawkins, Phillips Laboratory</i>
4:00 - 4:30	Progress Towards Synthesis of Pentaprismene and Bicyclopropylidene: Potential Rocket Fuel Additives <i>Dr. Suresh C. Suri, Hughes-STX Corporation</i>
4:30 - 5:00	Extra-High Energy Oxidizers and Fuels <i>Dr. Robert J. Schmitt, SRI International</i>
6:00 - 9:00	Poster Session, Reception

**Monday, 2 June 1997**

- 8:30 - 9:00            **New Methods for Excited States**  
*Dr. Rodney J. Bartlett, University of Florida*
- 9:00 - 9:30            **Theory and Synthesis of New High Energy Density Materials**  
*Dr. Karl O. Christe, Hughes STX Corporation*
- 9:30 - 10:00          **Synthesis of High-Energy Density Materials Based on Strained-Ring Compounds**  
*Dr. William P. Dailey, University of Pennsylvania*
- 10:00 - 10:30         *Break*
- 10:30 - 11:00         **Epoxidation Transition States and Stereoselectivity Modeling**  
*Dr. Kendall N. Houk, University of California, Los Angeles*
- 11:00 - 11:30         **Nitrogen Peroxides for HEDM Applications**  
*Dr. D. Scott Bohle, University of Wyoming*
- 11:30 - 12:00         **Models and Simulations of Energetic Materials**  
*Dr. Donald L. Thompson, Oklahoma State University*
- 12:00 - 1:30          *Lunch*
- 1:30 - 2:00            **The Role of Quantum Chemistry in the Design of High Energy Species**  
*Dr. Mark S. Gordon, Iowa State University*
- 2:00 - 2:30            **Reaction Field Cavity Optimization: A New Solvent Model for Electronic Structure Theory**  
*Dr. Teresa Head-Gordon, University of California, Berkeley*
- 2:30 - 2:45            **Direct Detection and Spectroscopy of  $O_4^+$**   
*Dr. Holly Bevsek, University of California, Berkeley*
- 2:45 - 3:15            *Break*

**Monday, 2 June 1997 (Cont'd)**

- 3:15 - 3:45      Computational Studies of High Energy Density Matter  
*Dr. Gregory A. Voth, University of Utah*
- 3:45 - 4:15      Spectral Theory of Physical and Chemical Binding:  
Aspects of Computational Implementation  
*Dr. Peter W. Langhoff, Indiana University*
- 4:15 - 4:45      Reactions of Laser-Ablated Boron Atoms with HCN. Infrared  
Spectra of BNC, BCN, HBNC and HBCN in Solid Argon.  
Reactions of Laser Ablated Aluminum Atoms with Ammonia.  
Infrared Spectra of  $\text{HAlNH}_2$ ,  $\text{AlNH}_2$  and  $\text{HAlNH}$  in Solid Argon  
*Dr. Lester Andrews, University of Virginia*
- TBD              Workshop - Theory/Synthesis  
Discussion Leader: *Dr. Jeffrey A. Sheehy, Phillips Laboratory*

**Tuesday, 3 June 1997**

- 8:30 - 9:00      Progress Towards the Production of Cryosolid HEDM Samples by  
Laser Ablation and Matrix Isolation Techniques  
*Dr. Mario Fajardo, Phillips Laboratory*
- 9:00 - 9:30      Characterization of Cryogenic Carbon and Boron HEDM  
*Dr. C. William Larson, Phillips Laboratory*
- 9:30 - 10:00     Theoretical Investigations of HEDM  
*Dr. Jeffrey A. Sheehy, Phillips Laboratory*
- 10:00 - 10:30    *Break*
- 10:30 - 11:00    Spectroscopy & Dynamics in Quantum Hosts  
*Dr. V. Ara Apkarian, University of California, Irvine*
- 11:00 - 11:30    Mass Spectrometry of Doped Helium Clusters  
*Dr. Kenneth C. Janda, University of California, Irvine*
- 11:30 - 12:00    Light Metal Atom Interactions with Hydrogen and Helium Clusters:  
Solvation Dynamics and Non-Adiabatic Effects  
*Dr. Kevin Lehmann, Princeton University*
- 12:00 - 1:30     *Lunch*

**Tuesday, 3 June 1997 (Cont'd)**

- 1:30 - 2:00      Spectroscopic Characterization of Non-Bonding Interactions of the Boron Atom  
*Dr. Paul J. Dagdigian, Johns Hopkins University*
- 2:00 - 2:30      Structure and Energetics of B(Ar)<sub>n</sub>, B(N<sub>2</sub>), and O(H<sub>2</sub>) Clusters  
*Dr. Millard H. Alexander, University of Maryland*
- 2:30 - 3:00      Fundamental Insights from HEDM Studies  
*Dr. David R. Yarkony, Johns Hopkins University*
- 3:00 - 3:30      *Break*
- 3:30 - 4:00      Calorimetric Measurements of O Atom Recombination  
*Dr. Peter Taborek and Dr. James E. Rutledge, University of California, Irvine*
- 4:00 - 4:30      Characterization of Metal Atom-Doped Cryogenic Solids  
*Dr. George M. Seidel, Brown University*
- 4:30 - 5:00      Ozone in Solid Oxygen  
*Dr. Richard A. Copeland, SRI International*
- 5:00 - 5:30      Advanced Cryogenic Solid Hybrid Rocket Engine Developments for HEDM and Non-HEDM Demonstrations  
*Mr. Eric E. Rice, Orbital Technologies Corporation (ORBITEC)*



**Tribology Program Review**  
**Holiday Inn, Englewood, Ohio**  
**24-26 June 1997**

**Tuesday, 24 June 1997**

- 0840        Introduction  
            *Major Hugh Delong, AFOSR, and Dr. Peter Schmidt, ONR*
- 0900        Soft and Hard Junctions. *Dr. Uzi Landman,*  
            *Georgia Institute of Technology*
- 0930        Kelvin Probe Measurements for Wear Monitoring,  
            *Dr. Steve Danyluk, Georgia Institute of Technology*
- 1000        Tribological Behavior of Polycrystalline Diamond and  
            Poly-/Single-Crystal Silicon in Vacuum and Hydrogen  
            for MEMS Micromechanism Applications,  
            *Dr. Michael N. Gardos, Hughes Aircraft Company*
- 1030        *Break*
- 1045        Fluorination of Diamond Surfaces by Irradiation of Adsorbed  
            Perfluorinated Alkyl Iodides. *Dr. John T. Yates, Jr.,*  
            *University of Pittsburgh*
- 1115        Nanotribological Studies of Bulk Ceramic Materials,  
            Multilayered Thin Films, and Liquid Lubricant Films,  
            *Dr. Bharat Bhushan, Ohio State University*
- 1145        Force Microscopy Studies of Tribology at the Nanometer Scale:  
            Probing the Molecular Origins of Friction. *Dr. Charles M. Lieber,*  
            *Harvard University*
- 1215        *Lunch*
- 1400        Tribology in Extreme Environments, *Dr. Jeff S. Zabinski, WL/MLBT*
- 1430        Advanced Carbon Based Coatings for Wear and Friction Reduction,  
            *Dr. Andrey A. Voevodin, WL MLBT*
- 1500        Lubricious Oxides. *Dr. Somuri V. Prasad, WL/MLBT*
- 1530        *Break*

- 1545 The Surface Chemistry and Tribology of Carbide and Nitride Hard Coatings, *Dr. Scott S. Perry, University of Houston*
- 1615 The Application of Raman Microscopy to the Friction, Wear and Tribochemistry of Solid Lubricating Films, *Dr. Larry E. Seitzman, Naval Research Laboratory*
- 1645 Tribological Studies Using the Surface Forces Apparatus (SFA) and the X-SFA, *Dr. Jacob Israelachvili, University of California, Santa Barbara*
- 1715 Electrostatic Charging Precursor to Scuffing in Lubricated Contacts, *Dr. Robert J. K. Wood, University of Southampton*

**Wednesday, 25 June 1997**

- 0830 Recent Progress Towards First-Principles Predictions of Fracture Strengths and Wear Resistance of Polycrystalline Covalent Ceramics, *Dr. Donald W. Brenner, North Carolina State University*
- 0900 Diffusion Mechanisms of Vapor Phase Lubricants, *Dr. Nelson H. Forster, WL POLS*
- 0930 Integrated Diagnostics, *Dr. Richard S. Cowan, Georgia Institute of Technology*
- 1000 *Break*
- 1015 Surface Treatments for Probing of Tribological State Variables, *Dr. Ursula Gibson, Dartmouth College*
- 1045 Temperature Probes for Detecting Incipient Failure of Tribological Components, *Dr. Francis E. Kennedy, Dartmouth College*
- 1115 A Thermal-Tribological Approach for Designing Tribological Elements and Its Applications to Engine Pistons and Journal Bearings, *Dr. Qian (Jane) Wang, Florida International University*
- 1145 New Spectroscopic and Theoretical Probes of Tribochemical Processes, *Dr. Dor Ben-Amotz, Purdue University*
- 1215 *Lunch*

- 1400 The Nature of Tribochemistry and the Effectiveness of BL Films,  
*Dr. Stephen M. Hsu, University of Maryland*
- 1430 Deformation Behavior of Thin Liquid Films at Elevated Pressure,  
*Dr. Scott Bair, Georgia Institute of Technology*
- 1500 High-Temperature Liquid Lubricant and Additive Research,  
*Dr. Harvey L. Paige, WL MLBT*
- 1530 *Break*
- 1545 Fundamental Studies of the Interactions of Perfluoropolyalkylether Based  
Fluids with Iron Containing Surfaces, *Dr. Jeffrey Sanders, WL MLBT*
- 1615 Nanorheology in the Service of Tribology with Emphasis on  
Perfluoroethers, *Dr. Steve Granick, University of Illinois*
- 1645 Tribological Properties of Molecular Monolayers on Metal  
Surfaces, *Dr. Andrew J. Gellman, Carnegie Mellon University*
- 1715 Materials Degradation and Fatigue Under Extreme Conditions,  
*Dr. Jiri Jonas, University of Illinois*

**Thursday, 26 June 1997**

- 0830 Nanoarches and Nucleation and Growth of Cubic Boron Nitride,  
*Dr. Laurence D. Marks, Northwestern University*
- 0900 Molecular Dynamics Investigations of the Tribology of Hydrocarbons,  
*Dr. Judith A. Harrison, US Naval Academy*
- 0930 Molecular Dynamics Simulations of Ceramics,  
*Dr. John W. Mintmire, Naval Research Laboratory*
- 1000 *Break*
- 1015 Variational Fitting and Quantum-Chemical Nanotribology,  
*Dr. Brett I. Dunlap, Naval Research Laboratory*
- 1045 Theory of Scanning Tunneling Microscopy (STM) Spectra Through  
Molecular Adsorbates: Investigating Charge Structure and Charge  
Flow at a Molecule Functionalized Metal Surface, *Dr. Mark Ratner,  
Northwestern University*

- 1115      Determining the Interactions Between Polymer-Coated Surfaces  
Through Theory and Simulation, *Dr. Anna C. Balazs,*  
*University of Pittsburgh*
- 1145      Lattice and Continuum Models of Some Mechanical Properties  
of S-P Metals and Directionally Bonded Semiconductors,  
*Dr.: Norman H. March, Oxford University*
- 1215      *Adjourn*

**Chronobiology and Neural Adaptation Program Review**  
**United States Air Force Academy**  
**Colorado Springs, Colorado**  
**18-20 September 1997**

**Thursday, 18 September 1997**

- 0730           Registration/Continental Breakfast
- 0830           Introduction  
*Dr. Genevieve Haddad, AFOSR*
- 0900           Organization of the Human Circadian System  
*Dr. Robert Y. Moore, University of Pittsburgh*
- 0930           PRET95 Homeostatic and Circadian Regulation of Wakefulness During  
Jet Lag and Sleep Deprivation: Effect of Wake-Promoting  
Countermeasures on the Development of Neurobehavioral Deficits  
*Dr. David F. Dinges, University of Pennsylvania School of Medicine*
- 1000           The Effect of Caffeine on the Circadian and Homeostatic Interaction  
Underlying the Deterioration of Neurobehavioral Functioning During Jet  
Lag and Sleep Deprivation  
*Dr. Derk-Jan Dijk, Brigham & Women's Hospital, Harvard Medical  
School*
- 1030           *Break*
- 1100           The Effect of Exercise on Endogenous Circadian Period, Sleep and  
Performance  
*Dr. Charles A. Czeisler, Brigham & Women's Hospital, Harvard  
Medical School*
- 1130           Circadian Phase Alters the Cost of Paying Attention  
*Dr. Jeremy Wolfe, Brigham & Women's Hospital, Harvard Medical  
School*
- 1200           *Break*
- 1215           Effects of Light, Exercise and Manipulations of the Sleep-Wake  
Cycle on Human Circadian Rhythms  
*Dr. Eve Van Cauter, University of Chicago*

- 1245      Circadian and Metabolic Modulation of Human Vision  
*Dr. Robert B. Barlow, SUNY Health Science Center*
- 1315      *Lunch*
- 1430      Air Force Basic Research Program on Human Chronobiology and Sleep  
*Dr. Rod J. Hughes, Air Force Research Laboratory, Brooks AFB*
- 1500      Crew Fatigue During Simulated, Long Duration B-1B Bomber Missions  
*Dr. Jonathan French, Air Force Research Laboratory, Brooks AFB*
- 1530      Verbal Communication in Team Situational Awareness  
*Dr. Linda R. Elliott, Air Force Research Laboratory, Brooks AFB*
- 1600      *Break*
- 1615      Learning Abilities Measurement Program. Individual Differences  
*Dr. Pat Kyllonen, Air Force Research Laboratory, Brooks AFB*
- 1645      Individual Differences in Diurnal Preference  
*Dr. Richard D. Roberts, Air Force Research Laboratory, Brooks AFB*
- 1715      EEG Pattern Recognition of Individual Differences in Cognitive Abilities  
*Dr. Alan Gevins, SAM Technology*
- 1900      *Dinner at Officers Club*
- 1945      **Air Force Operational Viewpoint.** Speaker, *Col Dale Hammer,*  
*United States Air Force Academy, Colorado Springs*

**Friday, 19 September 1997**

- 0830      Continental Breakfast
- 0900      Control of Circadian Behavior by Transplanted Suprachiasmatic Nuclei  
*Dr. Michael Menaker, University of Virginia*
- 0930      Dissecting the Mammalian SCN  
*Dr. Rae Silver, Columbia University*
- 1000      *Break*
- 1015      Neural Stem Cells - Transplantation and the Circadian System  
*Dr. William J. Schwartz, University of Massachusetts Medical School*

- 1045      Organization Within and Among Vertebrate Circadian Oscillators  
*Dr. Gene D. Block, University of Virginia*
- 1115      *Break*
- 1130      Cellular Analysis of Circadian Rhythmicity in Cultured SCN Neurons  
*Dr. Steven M. Reppert, Massachusetts General Hospital*
- 1200      Intracellular Electrophysiology of the Rat Suprachiasmatic Nucleus:  
 Membrane Properties, Neurotransmission and Effects of  
 Neuromodulators  
*Dr. F. Edward Dudek, Colorado State University*
- 1230      *Lunch*
- 1400      Modulation of Neuronal Activity in the Suprachiasmatic Nucleus  
*Dr. Anthony N. van den Pol, Yale University Medical School*
- 1430      Synaptic Plasticity and Memory Formation Modifying the Operation of  
 AMPA-Type Glutamate Receptors: Memory Encoding and a Novel  
 Pharmacology  
*Dr. Gary Lynch, University of California, Irvine*
- 1500      *Break*
- 1515      Dynamic Reconfiguration of a Pattern Generating Neural Network  
*Dr. John H. Byrne, University of Texas-Houston Health Science Center*
- 1545      Gene Regulation in Memory Formation and Circadian Rhythm  
*Dr. Arnold Eskin, University of Houston*
- 1700      Macaroni Grill

**Saturday, 20 September 1997**

- 0830      Continental Breakfast
- 0900      Neurophysiological and Behavioral Analysis of Circadian Rhythm  
 Entrainment  
*Dr. Benjamin Rusak, Dalhousie University*
- 0930      Neural Regulation of Non-Photic Entrainment  
*Dr. Lawrence P. Morin, Stony Brook University*
- 1000      *Break*

- 1015      Neurochemical Regulation of Circadian Phase  
*Dr. Michael A. Rea, Air Force Research Laboratory, Brooks AFB*
- 1045      Different Areas of the Brain May be Involved in Fear vs. Anxiety  
*Dr. Michael Davis, Yale University*
- 1115      PRET95 Homeostatic and Circadian Regulation of Wakefulness During  
Jet Lag and Sleep Deprivation: Effect of Wake-Promoting  
Countermeasures. Pre-Clinical Assessment of Compensatory Sleep  
Responses to Drug-Induced Waking  
*Dr. Dale M. Edgar, Stanford University*
- 1145      *Lunch*
- 1300      Interaction of Light and Clock Regulation in Neurospora  
*Dr. Jennifer J. Loros, Dartmouth Medical School*
- 1330      Probing the *Drosophila* Circadian System Using Enhancer Detectors  
*Dr. Paul E. Hardin, University of Houston*
- 1400      *Break*
- 1430      Circadian Rhythms in Zebrafish and Genetic Analysis of Vertebrate  
Circadian Rhythmicity  
*Dr. Gregory M. Cahill, University of Houston*
- 1500      Genetic Analysis of Daily Activity in Humans and Mice  
*Dr. Joseph S. Takahashi, Northwestern University*
- 1530      *Closing Remarks*
- 1800      Chuckwagon Suggest at Flying W Ranch



# **AFOSR/ONR Electrochemistry Science & Technology Review**

**Doubletree Hotel, Ventura, California  
15-16 January 1998**

**Thursday, 15 January 1998**

- 0700           Registration/Continental Breakfast
- 0800           Introduction  
*Dr. Richard T. Carlin, ONR, and Dr. Hugh C. De Long, AFOSR*
- 0815           Nanocomposite Polymer Electrolytes, *Dr. Emmanuel P. Giannelis, Cornell University*
- 0840           Properties of Fuel Cell and Battery Materials, *Dr. P. E. Stallworth, Dr. John J. Fontanella, Dr. M. C. Wintersgill, Dr. C. A. Edmondson, U. S. Naval Academy*
- 0905           NMR Investigations of Materials for Batteries & Fuel Cells, *Dr. Steve Greenbaum, Hunter College of CUNY*
- 0930           Polymeric Gels as an Environment for Electrochemistry, *Dr. Malgorzata Ciszewska, Brooklyn College*
- 0950           Low Dimensional Fast Ion Conductors, *Dr. Larry G. Scanlon, Air Force Research Laboratory*
- 1015           *Break*
- 1030           Single Lithium Ion Conducting Polymer Electrolyte, *Dr. William A. Feld, Wright State University*
- 1055           Synthesis of a Mesomorphic, Columnar Porphyrin for Fast Li Ion Conducting Electrolytes, *Dr. John Arnold, University of California, Berkeley*
- 1120           X-Ray Absorption Structural and Electrochemical Studies of Novel Materials for Advanced Batteries and Ultracapacitors, *Dr. Azzam N. Mansour, Naval Surface Warfare Center*

- 1140 Remediation of Aqueous Waste by Electrified Microheterogeneous Catalysis. *Dr. Debra Rolison, Naval Research Laboratory*
- 1205 *Lunch*
- 1330 Electrochemical Properties of Sol-Gel Derived Materials, *Dr. Bruce Dunn, University of California, Los Angeles*
- 1355 Electroanalytical Investigations of Sol-Gel Derived Materials, *Dr. Maryanne M. Collinson, Kansas State University*
- 1420 Development of New Trace Analytical Capabilities at the Electrode/Solution Interface and Their Application to a Novel Thin Film Battery System. *Dr. Daniel A. Buttry, University of Wyoming*
- 1445 Clay-Templated Nanoporous Graphitic Carbon Electrodes for Secondary Batteries. *Dr. Mahmoud Aldissi, Dr. E. Lazaro, Dr. M. Bhamidipati and Dr. B. Dixon, Cape Cod Research*
- 1510 *Break*
- 1525 Nanofibrils Carbon Electrode for Rechargeable Batteries, *Dr. Chuanjing Xu, Nanomaterials Research Corporation*
- 1550 Composite Nanoscale Cathodes for Li-Ion Batteries, *Dr. Michael C. Kimble, Physical Sciences, Inc.*
- 1615 Electrocatalysts Based on Electrode-Confined Dendrimers, *Dr. Richard M. Crooks, Texas A&M University*
- 1640 The Solution Phase Catholyte Semi Fuel Cell Utilizing a Flowing Aqueous Electrolyte, *Dr. Eric G. Dow and Dr. Maria G. Medeiros, Naval Undersea Warfare Center*
- 1700 Electrode Surface Modification for Cathode Catalysis in Semi-Fuel Cells, *Dr. Russell R. Bessette and Dr. James M. Cichon, University of Massachusetts, Dartmouth*
- 1725 *Break*
- 1800 Semi-Fuel Cell Mini-Symposium

**Friday, 16 January 1998**

- 0745 Continental Breakfast
- 0825 Probing Step Density Effects on Reactions at Single Crystal Electrodes,  
*Dr. Carol Korzeniewski, Texas Tech University*
- 0850 Electrodeposition Dynamics and Redox Probe Microscopy,  
*Dr. Hector D. Abruna, Cornell University*
- 0915 Phase Dynamics and Rate/Structure Correlations in Electrocatalytic  
Nanoclusters. *Dr. Ralph G. Nuzzo, Dr. John R. Shapley, Dr. Anatoly I.  
Frenkel, Dr. Michael S. Nashner, and Dr. Charles W. Hills,  
University of Illinois, Urbana-Champaign*
- 0940 Metallic Monolayers as Fuel Cell Electrode Catalysts,  
*Dr. Stanley D. James, Naval Surface Warfare Center*
- 1000 *Break*
- 1015 New Opportunities in Fundamental Nanoelectrochemistry and  
Bioelectrochemistry, *Dr. Charles R. Martin, Colorado State University*
- 1040 Studies of Latent Acidity and Neutral Buffered Chloroaluminate Ionic  
Liquids, *Dr. Robert A. Osteryoung, North Carolina State University*
- 1105 Developing Lithium Thermal Batteries for Navy and Joint-Service Air-  
Launched Weapons, *Dr. Carl H. Hinners, Naval Air Warfare Center*
- 1125 Applications of Ambient-Temperature Ionic Liquids to Compact Power  
Sources and Electrodeposition of Advanced Aluminum Alloys,  
*Dr. Paul C. Trulove, U. S. Naval Academy*
- 1150 Double Layer Studies at Single-Crystal Electrodes in Non-Aqueous  
Solutions, *Dr. W. Ronald Fawcett, University of California, Davis*
- 1215 *Lunch*
- 1330 Two Facets of Electron Transfer: Solvent Dynamics and Charge Transfer,  
Electron-Molecule Collision Insight into Organic Halide Anion Potential  
Energy, *Dr. Rudolph A. Marcus, California Institute of Technology*
- 1355 Electron Transfer at Nanoscale Electrochemical Interfaces,  
*Dr. Joseph T. Hupp, Northwestern University*

- 1420 Charge Transfer Systems of Molecular Dimensions, *Dr. Royce W. Murray, University of North Carolina*
- 1445 The Response of Water in High Surface Electric Fields.  
*Dr. Eric M. Stuve, University of Washington*
- 1510 Electrochemical-Engendered Convective Transport in Magnetic and  
Electric Fields, *Dr. Henry S. White, University of Utah*  
1535 *Break*
- 1550 Electrochemical Growth of Heteroepitaxial Layers of Low-Dimensional  
Conductors, *Dr. Daniel E. Hooks and Dr. Michael D. Ward, University of Minnesota*
- 1615 Catecholamine Secretion from Single Cells. *Dr. R. Mark Wightman, University of North Carolina at Chapel Hill*
- 1640 Understanding the Mechanism of Ennoblement of Stainless Steels,  
*Dr. Zbigniew Lewandowski, Montana State University*
- 1705 A Hybrid Electrochemical/Chemical Method for the Epitaxial Synthesis of  
Compound Semiconductor Nanocrystallites on Graphite,  
*Dr. Reginald M. Penner, University of California, Irvine*
- 1730 Electrochemical Assembly of Nanophase Metal Oxides.  
*Dr. Jay A. Switzer, University of Missouri, Rolla*
- 1755 Polymerized Phthalocyanines for Electrochemical Applications,  
*Dr. Peter W. Faguy, University of Louisville*
- 1820 *Closing Remarks*

## AGENDA

### 2<sup>nd</sup> Annual Review of AFOSR MURI "Nanoscale Devices and Novel Engineered Materials"

University of Florida

Monitor: Maj. H.C. DeLong, Ph.D.

Tuesday

February 17, 1998

Location: Coral Room A, Holiday Inn Sun Spree Resort  
Clearwater Beach, Florida

9:00 am Welcome and Overview of Program -- S.J. Pearton (MSE/UF)  
9:15 am Program Goals and Achievements -- J.R. Childress (MSE/UF)

#### Novel Engineered Materials and Properties

9:30 am Nanoparticle Dispersions in Polymer Matrices -- E.P. Goldberg (MSE/UF)  
10:00 am COFFEE BREAK  
10:30 am Porous Si -- R.E. Hummel (MSE/UF)  
11:20 am Molecular Cluster Calculations on Display Materials -- J. Lewis (MSE/UF)  
11:35 am Pulsed Laser Deposition of Nanoparticle  $Y_2O_3:Eu$  -- S. Jones (MSE/UF)  
12:00 Noon LUNCH  
1:30 pm Mechanical Properties of Nanostructured Materials -- S.A. Syed Asif (NRL)

#### Advanced Nanostructures

2:00 pm Quantum Effects in Magnetic and Superconducting Materials -- L.K. Schuller  
(Physics/UCSD)  
2:45 pm COFFEE BREAK  
3:15 pm Integration of Magnetic Nanoparticles with 2D Electron Systems -- S. von Molnar  
(Physics/FSU)  
4-5:30 pm Discussion (all)

Wednesday

February 18, 1998

Location: Coral Room A

#### Submicron Magnetic Structures: Theory, Deposition and Processing

9:00 am Overview -- J.R. Childress (MSE/UF)  
9:15 am Nanoscale Patterning -- F. Sharifi (Physics/UF)  
10:00 am Novel Magnetoresistive Materials -- J.R. Childress (MSE/UF)  
10:45 am COFFEE BREAK  
11:15 am Fabrication, Deposition and Characterization in Support of Magnetic Sensor  
Development -- D. Temple (MCNC)  
12:00 Noon LUNCH  
1:30 pm Theory & Modelling of GMR -- S. Hershfield (Physics/UF)  
2:15 pm Dry Etching of Magnetic Materials -- S.J. Pearton (MSE/UF)  
3:00 pm COFFEE BREAK  
2:30-4:00 pm Summary/Future Plans -- S.J. Pearton (MSE/UF)  
4-5:30 pm Discussion (all)

# AFOSR COMPOSITE DURABILITY WORKSHOP

9 October 1997

Dearborn Inn, Dearborn, MI

730 Continental Breakfast

830 Charles Lee

845 Ozden Ochoa

900 Morgan

915 Yee

930 Leung

945 coffee break

1000 Seferis

1015 Curliss

1030 Reifsnider

1045 Piggott

1100 Kumosa

1115 Whitcomb

1130 Daniel

1145 Lunch

1300 Round Table Discussion

1400 break

1700 adjourn latest

## AGENDA

### Air Force New World Vistas "People" Research

Kick-off Meeting  
16-May-97

0830 CONVENE AT SALON B, MARRIOTT RIVERWALK HOTEL, SAN ANTONIO TX

0830 Dr. Brendan Godfrey AF Armstrong Laboratory  
Welcome/Introduction

0845 Dr. John F. Tangney AF Office Scientific Research  
Program Overview

0900 Dr. Linda R. Elliott AF Armstrong Lab  
Distributed Team Decision-Making and Performance  
in Complex Environments

0915 Dr. Elizabeth Martin AF Armstrong Laboratory  
Uninhabited Combat Air Vehicle (UCAV) Training Research Testbed

0930 Dr. Ellen Hall AF Armstrong Laboratory  
Cognitive Engineering for Team Tasks

0945 Dr. Alan S. Gevins SAM Technology  
EEG-Based Online Cognitive Load Monitor

1000 BREAK

1020 Dr. Michael W. Haas AF Armstrong Laboratory  
Understanding Attentional Mechanisms Underlying Increases  
in Performance Associated with Multi-Dimensional Displays

1035 Dr. Robert H. Glick Wright State University  
Cognitive Workload in a Complex Synthetic Task Environment:  
The Role of Functional Display and Control Representations

1050 Dr. Phillip L. Ackerman University of Minnesota  
Cognitive Modeling and Task Analysis

1105 Dr. F. Javier Lerch Carnegie Mellon University  
Integrated Cognitive, Computational and Biological Assessment  
of Workload in Decision Making

1120 Dr. Wes Regian AF Armstrong Laboratory  
Training Research for Automated Instruction (TRAIN)

1135 ADJOURN 13-May-97

## **AFOSR DURABLE COATINGS PANEL REVIEW**

Room 354, Polymer Branch  
Building 654  
Wright-Patterson AFB, OH

20 May 1997

- 0830 Closed Meeting  
*Government and Advisors Only*
- 0900 Opening Remarks  
*Charles Y-C Lee, AFOSR*
- 0915 ML Coating Effort  
*Arnold Donley, Wright-Patterson AFB*
- 0945 ML 6.1 Effort  
*Fred Arnold, Wright-Patterson AFB*
- 1015 *Break*
- 1030 Dharmaraj Raghavan  
*Howard University*
- 1100 Mark Soucek  
*North Dakota State University*
- 1130 Yanching Jean  
*University of Missouri - Kansas*
- 1200 *Lunch*
- 1300 J. R. Reynolds  
*University of Florida*
- 1330 Paras Prasad  
*SUNY at Buffalo*
- 1400 Thomas Serry  
*University of Connecticut*
- 1430 General Discussions/Adjournment



May 22, 1997

**SUMMARY OF REVIEWS**  
**AFOSR Molecular Dynamics Panel Meeting**

- 97-NL-102      Ion and Neutral Dynamics of Ceramic Materials Formation and Atmospheric Processes**  
- Stephen R. Leone, University of Colorado
- Laurie J. Butler, University of Chicago (A-/2/3)  
Steven D. Colson, Pacific Northwest National Laboratory (A+/2)  
Charles S. Parmenter, Indiana University (A/A+/3)  
James C. Weisshaar, University of Wisconsin (A/1)  
J. Michael White, University of Texas at Austin (A/B+/3)
- 97-NL-137      The Growth of Nanostructures and Composite Films on Solids: Simulations and Phenomenological Theory**  
- Hona L. Metiu, University of California
- Jeffrey Hay, Los Alamos National Laboratory (A/3)  
Hannes Jonsson, University of Washington (A+/1)  
Max G. Lagally, University of Wisconsin-Madison (A-/2)  
J. Michael White, University of Texas at Austin (A+/3/4)
- 97-NL-152      Theoretical Studies of Group IVA and Group IVB Chemistry**  
- Mark S. Gordon, Iowa State University
- Christopher J. Cramer, University of Minnesota (A+/1)  
Larry Harding, Argonne National Laboratory (A/3)  
Jeffrey Hay, Los Alamos National Laboratory (A/1)  
George Schatz, Northwestern University (A/1)  
Jack Simons, University of Utah (A-/1)
- 97-NL-153      Study of Complex Kinetic Systems with Imposed Variation of Temperature**  
- John Ross, Stanford University
- William L. Hase, Wayne State University (B/4)  
Jeffrey Hay, Los Alamos National Laboratory (\*/5)  
Joel E. Keizer, University of California, Davis (B/B+/1)  
Davis W. Oxtoby, University of Chicago (A/3)  
George Schatz, Northwestern University (A/3)
- \*Note: Letter grade not given.**

- 97-NL-156 Femtosecond Dynamics of Chemical Reactions**  
 - Almed H. Zewail, California Institute of Technology
- Laurie J. Butler, University of Chicago (A-/2)  
 Steven D. Colson, Pacific Northwest National Laboratory (A+/2)  
 Edward R. Grant, Purdue University (A+/3)  
 Charles S. Parmenter, Indiana University (A-/3)  
 James C. Weisshaar, University of Wisconsin (A/4)
- 97-NL-157 Microwave Cavity Spectroscopy**  
 - Richard N. Zara, Stanford University
- Laurie J. Butler, University of Chicago (A-/2/4)  
 Steven D. Colson, Pacific Northwest National Laboratory (A-/3)  
 Paul L. Houston, Cornell University (A-/3)  
 Charles S. Parmenter, Indiana University (A-/3/4)  
 James C. Weisshaar, University of Wisconsin (A/3)
- 97-NL-158 Dynamical Spectroscopy of Prototypes in Condensed Phase Chemistry**  
 - V. Ara Apkarian, University of California
- Laurie J. Butler, University of Chicago (A/2/5)  
 Charles S. Parmenter, Indiana University (A/A-/4/5)  
 George Schatz, Northwestern University (A/2)  
 Norbert F. Scherer, University of Pennsylvania (A/A/1)  
 James C. Weisshaar, University of Wisconsin (B+/5)
- 97-NL-159 Energy Transfer Kinetics and Dynamics of Relevance to Iodine Lasers**  
 - Michael C. Heaven, Emory University
- Laurie J. Butler, University of Chicago (A-/B+/2)  
 Steven D. Colson, Pacific Northwest National Laboratory (B+/3)  
 John B. Koffend, Los Angeles (A-/1)  
 Charles S. Parmenter, Indiana University (B+/2)  
 James C. Weisshaar, University of Wisconsin (A-/3)
- 97-NL-160 Theoretical Studies of Gas Phase Elementary Reactions**  
 - Keiji Morokuma, Emory University
- Clifford E. Dykstra, Indiana University, Purdue (A-/2/3)  
 William L. Hase, Wayne State University (A/2)  
 Jeffrey Hay, Los Alamos National Laboratory (A/1)  
 George Schatz, Northwestern University (A-/1)  
 Jack Simons, University of Utah (A-/1)

**97-NL-161      Electronic, Phonon and Optical Properties of the Polyhedral Cage Materials:  
Si and Ge Clathrates**

- Peter C. Eklund, University of Kentucky

Sanford A. Asher, University of Pittsburgh (B+/4)

Steven D. Colson, Pacific Northwest National Laboratory (A/4)

Robert L. Whetten, Georgia Institute of Technology (A+/2)

J. Michael White, University of Texas at Austin (A-/4)

**97-NL-166      Atomistic Simulations of High-Temperature Ceramics Metal/Ceramic  
Interfaces, and MEMS on Parallel Computers**

- Rajiv K. Kalia, Louisiana State University

Donald E. Ellis, Northwestern University (A/1)

Jeffrey Hay, Los Alamos National Laboratory (A-/2)

John Mintmire, Naval Research Laboratory (A/1)

George Schatz, Northwestern University (A/3)

J. Michael White, University of Texas at Austin (A-/3/4)

**97-NL-169      Fundamental Studies of Ions and Ionic Processes**

- Henry F. Schaefer III, University of Georgia

Clifford E. Dykstra, Indiana University-Purdue (A/1/2)

Jeffrey Hay, Los Alamos National Laboratory (A-/1)

J. Vince Ortiz, Kansas State University (A/2)

George Schatz, Northwestern University (A-/A/1)

November 6, 1997

**SUMMARY OF REVIEWS**  
**AFOSR Molecular Dynamics/Theoretical**  
**Chemistry Review Panel Meeting**

- 97-NL-172 Intramolecular Vibrational Energy Transfer and Bond-Selected Photochemistry in Liquids**  
- F. Fleming Crim, University of Wisconsin
- Laurie J. Butler, University of Chicago (A-/2)  
Hai-Lung Dai, University of Pennsylvania (A-/3)  
George W. Flynn, Columbia University (A/2)  
Charles S. Parmenter, Indiana University (A/2)
- 97-NL-342 Linear Scaling Density Functional Theory With Periodic Boundary Conditions**  
- Gustavo E. Scuseria, Rice University
- Michael Colvin, Lawrence Livermore Laboratories (A/2)  
Richard A. Friesner, Columbia University (A/1)  
Peter M.W. Gill, University of Cambridge, UK (B+/1)  
Jeffrey Hay, Los Alamos National Laboratory (A-/2)  
George C. Schatz, Northwestern University (A/2)
- 97-NL-346 Electronic Processes Governing Non-Adiabatic Photodissociations and Chemical Reactions**  
- Karl F. Freed, The University of Chicago
- Ernest R. Davidson, Indiana University (A-/1)  
Jeffrey Hay, Los Alamos National Laboratory (A-/2)  
Morris Krauss, CARB/NIST (A/1)  
George C. Schatz, Northwestern University (A/2)  
Donald G. Truhlar, University of Minnesota (A/1)
- 97-NL-356 Stability, Growth and Reactivity at High Temperature Intermetallic Surfaces**  
- Talat S. Rahman, Kansas State University
- Charles T. Campbell, University of Washington (B+/3)  
Steven D. Colson, Pacific Northwest National Laboratory (A-/4)  
Bruce E. Koel, University of Southern California (B+/3)  
J. Michael White, University of Texas at Austin (A/3)

**97-NL-361 "Reactive" Vibrational Relaxation in the Gas-Phase and on Surfaces**

- Alec M. Wodtke - University of California

Laurie J. Butler, University of Chicago (A-/2)

Steven D. Colson, Pacific Northwest National Laboratory (A/3)

Paul L. Houston, Cornell University (A/1)

Charles S. Parmenter, Indiana University (A/2)

James C. Weisshaar, University of Wisconsin (A/2)

**97-NL-362 Controlled Forward and Inverse Chemical Dynamics**

- Herschel Rabitz, Princeton University

Paul W. Brumer, University of Toronto (A-/1)

David Hoffman, Iowa State (A/3)

Stuart A. Rice, University of Chicago (A/1)

George C. Schatz, Northwestern University (A/2)

**97-NL-364 Simulation of Reaction Dynamics: Nonadiabatic and Solvation Effects**

- Sharon Hammes-Schiffer, University of Notre Dame

Jeffrey Hay, Los Alamos National Laboratory (A/3)

Edward F. Hayes, Ohio State University (B/2-3)

Anne B. McCoy, Ohio State University (B+/4)

George C. Schatz, Northwestern University (A/1)

Donald G. Truhlar, University of Minnesota (A+/1)

James C. Weisshaar, University of Wisconsin (A/4)

J. Michael White, University of Texas at Austin (?/4)

**97-NL-369 Dynamics of Molecule-Surface Interactions on Metal Oxides**

- Curt Wittig, University of Southern California

Laurie J. Butler, University of Chicago (A/2/3)

Steven D. Colson, Pacific Northwest National Laboratory (A+/3)

Charles S. Parmenter, Indiana University (A-/4)

Charles T. Rettner, IBM Almaden Research Center (A/1)

James C. Weisshaar, University of Wisconsin (A/3)

J. Michael White, University of Texas at Austin (A+/1)

97-NL-417    **Experiments in Molecular Optics**  
- Robert J. Gordon, University of Illinois, Chicago

Laurie J. Butler, University of Chicago (A+/A/A-/3)  
Steven D. Colson, Pacific Northwest National Laboratory (A-/3)  
Charles S. Parmenter, Indiana University (A/4)  
George C. Schatz, Northwestern University (A/3)  
James C. Weisshaar, University of Wisconsin (A/3)

## **STTR PROGRAM REVIEW**

February 3, 1998

Meeting Room II

Holiday Inn Conference Center

Dayton, Ohio

8:30 - 8:45	Government Only Session
9:00	Open Session Begins
9:00 - 9:15	Comments by Charles Lee (Topic Manager) and Chris Hughes (STTR Manager at AFOSR)
9:15- 9:45	Sentel Technologies-EO Fiber
9:45-10:15	F&S-Ionic Self Assembly Monolayer
10:15-10:45	Break
10:45-11:15	PD-LD-Self Assembly Organical Chemical Beam Deposition
11:15-11:45	Pacific Wave Industries-New Directions in NLO Materials
11:45-12:15	Los Gatos Research-NLO Thin Film for Inspection
12:15-13:15	Lunch
13:15-13:45	Optivision-Development of In-line Fiber Devices
13:45-14:15	EIC Laboratories-Regioregular NLO Polymers
14:15-14:45	MetroLaser, Inc.-Novel Organic Film for Real Time Holographic Signal Processing
14:45-15:15	Break
15:15	Closed Session Begins
15:15-15:45	Cornerstone-Glass Forming LC for Photonic Devices
15:45-16:45	Government Only Session

## APPENDIX M



# **ANNUAL REPORT**

## **CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM**

**CONTRACT NO. F49620-95-C-0026**

**Period of Performance: 3/1/98 - 2/28/99**

### **Prepared For:**

**AIR FORCE OFFICE OF SCIENTIFIC RESEARCH  
CHEMISTRY AND LIFE SCIENCES DIRECTORATE**

**Dr. Genevieve Haddad, Program Manager**

### **Presented By:**

**UES, Inc.  
4401 Dayton-Xenia Road  
Dayton, OH 45432-1894**

## **INTRODUCTION**

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology; Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The third option year included: 66 Proposals that were reviewed;  
3 Program/Contractor Reviews; 3 Workshops and 1 Panel Meeting.

### **A. Evaluations of Individual Research Proposals**

UES sent out 66 proposals to 196 evaluators during the performance period of 1 March 1998 through 28 February 1999.

UES has been providing the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is now being sent electronically as well as a hard copy. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

### **B. Contractor/Program Reviews**

1. The first program review was joint and entitled **Molecular Dynamics (MD) and High Energy Density Matter (HEDM)**. It was held 17-22 May 1998 at the Hyatt Regency in Monterey, CA. Of the 143 attendees, 58 were speakers. These two meetings were held consecutively to stimulate interactions between program participants, and to expose AFOSR investigators to the wide range of topics being addressed in Air Force programs. Recent advances and accomplishments of the program were outlined at these

meetings. UES acquired the meeting site and made all arrangements for the meeting including meals and audio visual equipment. UES also provided on-site support and one advisor for the MD portion of the meeting.

*Dr. Michael Berman, Program Manager*

2. The second program review was a joint AFOSR/ONR/NSF **Tribology** review encompassing a wide range of topics: lubricants, wear resistant coatings, synthesis, characterization, modeling, simulations, metals, ceramics, polymers, etc. It was a broad-brush approach to the area and represented most of the tribology funded in the USA. This joint meeting brought together in one place all PI's funded in tribology to allow for cross-fertilization to take place. It also allowed the program managers to look at the programs as a whole, assess impacts, and possible new directions needed. It was deemed invaluable to the program managers as a source of what research the community is performing. This joint meeting provided participants insight into what the other participants are contributing and how and provided the opportunity for new collaborations between attendees. It was held 22-25 June 1998 at the Lowes Annapolis Hotel in Annapolis, MD. Of the 61 attendees, 49 were speakers.

*Major-Hugh De Long, Program Manager*

3. The third program review was **MURI and Durable Coatings**. It was held 11-22 January 1999 at Hawk's Cay Resort and Marina in Duck Key, Florida. There were 78 in attendance of which 59 were speakers. UES provided travel and per diem for 6 reviewers. UES also provided on-site support, made all arrangements for the meeting including meals and audio visual equipment.

*Major Hugh De Long, Program Manager*

### **C. Workshops**

1. The first workshop was a **Night Ops Working Group** workshop. It was held at Charleston AFB, SC on 28-29 May 1998. UES provided 9 advisors for the subject workshop and made arrangements for coffee breaks.

*Dr. Genevieve Haddad, Program Manager*

2. The second workshop was entitled **Polymer Composites**, and was held at the Anaheim Hilton & Towers in Anaheim, CA on 5 June 1998. UES made arrangements for the meeting location, audio visual and coffee breaks.

*Dr. Charles Lee, Program Manager.*

3. The third workshop was entitled **POSS Polymers** and was held at Sommerfield Suites, El Segundo, CA on 16 February 1999. Approximately 8-12 were in attendance. UES made arrangements for the meeting location, audio visual and beverages.

*Dr. Mike Berman, Program Manager*

#### **D. Panel Meeting**

The **Phase I STTR** panel meeting was held 18-19 February 1999 at Holiday Inn I 675 in Fairborn, OH. The purpose of this workshop was to hold a Phase I progress review to facilitate selection of Phase I efforts for submitting Phase II proposals for Phase II competition. Adhesives, flexible electronics and photonics were reviewed. There were ten presenters. UES made arrangements for the meeting room, audio visual equipment and coffee breaks.

*Dr. Charles Lee, Program Manager*

#### **E. Advisors**

In addition to advisors provided for Program Reviews, Workshops and Panel Meetings, UES provided travel, per diem and in many cases, honorarium for the following advisors:

Peter Stang and Frank Bates, **Nanostructures**, University of Southern California, Berkeley, CA, 9-10 March 1998.

Pat Hagans, **Corrosion Symposium**, Electrochemical Society Meeting, San Diego, CA, 3-8 May 1998.

Eileen Kowler and David Kieras, **Advisors on Human Performance**, George Mason University, Fairfax, VA, 26 May 1998.

Joan Fuller, **European Research Conference on Molten Salts**, Porquerolles, FR, 27 Jun – 3 Jul 1998.

Torbjorn Akerstedt, **AFOSR PRET Meeting**, Brigham & Women's Hospital, Boston, MA, 17 Jul 1998.

Ray Taylor, **Workshop on Advanced Metal Finishing Techniques for Aerospace Applications**, Keystone Resort, Keystone, CO, 23-28 Aug 1998.

Stephen Davis, **Workshop on Chemical Laser**, Albuquerque, NM, 16-18 Sep 1998.

Willard Larkin, **Technical Advisor to AFOSR**, Arlington, VA, 1 Oct – 31 Dec 1998.

Roger Brooks and Richard Goris, **AFOSR MURI Workshop in Infrared Biosensors**, University of Texas, Austin, TX, 2-3 February 1999.

## **SUMMARY**

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Thomas Eggemeier as Program Manager, Judith M. Flory, Program Administrative Manager, Donna Tinley, Assistant Program Administrator and Ann Corbitt as Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

## **LIST OF APPENDICES**

Breakdown of Research Proposals by Program Manager

Program for Molecular Dynamics Contractor's Meeting, Naval Postgraduate School and Hyatt Regency Monterey, Monterey, CA, 17-20 May 1998

Program for High Energy Density Matter Contractor's Meeting, Naval Postgraduate School and Hyatt Regency Monterey, Monterey, CA, 20-22 May 1998

Program for Night Operations Working Group Site Visit, 437<sup>th</sup> Airlift Wing, Charleston AFB, SC, 27-29 May 1998

Program for AFOSR/ONR/NSF Tribology Program Review, Lowes Annapolis Hotel, Annapolis, MD, 22-25 June 1998

Programs for MURI and Durable Coatings Program Reviews, Hawk's Cay Resort and Marina, Duck Key, Florida, 11-21 January 1999

Program for STTR Program Review, Holiday Inn Conference Center I-675, Fairborn, OH, 18-19 February 1999

## **BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER**

<u>PROGRAM MANAGER</u>	<u>NO. OF PROPOSALS</u>
Berman	17
De Long	6
Kozumbo	5
Larkin	1
Lee	19
Roach	8
Tangney	10

**1998 Molecular Dynamics Contractor's Meeting**  
**Naval Postgraduate School and**  
**Hyatt Regency Monterey**  
**Monterey, CA**  
**17-20 May 1998**

**Sunday, 17 May 1998**

- |                |  |
|----------------|--|
| 5:00 - 7:00 PM | Registration   |
| 7:00 - 7:15 PM | Introductory Remarks<br><i>Dr. Michael Berman, AFOSR</i>   |
| 7:15 - 7:45 PM | Ion Processes in the Upper Atmospheric and Space Environments<br><i>Dr. Rainer A. Dressler, AFRL, Hanscom AFB</i>      |
| 7:45 - 8:15 PM | Potential Energy Surfaces and Their Dynamic Implications<br><i>Dr. Keiji Morokuma, Emory University</i>                |
| 8:15 - 8:45 PM | Reactive Scattering of Atomic Oxygen on Hydrocarbon Surfaces<br><i>Dr. Timothy K. Minton, Montana State University</i> |
| 8:45 - 9:00 PM | Numerical Spectral Pattern Recognition<br><i>Dr. Matthew P. Jacobson, Massachusetts Institute of Technology</i>        |

**Monday, 18 May 1998**

- |                  |   |
|------------------|---|
| 8:45 - 9:15 AM   | Program Overview and Update<br><i>Dr. Michael Berman, AFOSR</i>   |
| 9:15 - 9:45 AM   | Reactivity of Air Plasma Ions with Hydrocarbon Fuel Components<br><i>Dr. Robert A. Morris, AFRL, Hanscom AFB</i>                          |
| 9:45 - 10:15 AM  | State-Resolved Ion Reactions and Ultrafast Photoelectron Spectroscopy<br><i>Dr. Stephen R. Leone, University of Colorado</i>              |
| 10:15 - 10:45 AM | <i>Break</i>  |
| 10:45 - 11:15 AM | Cavity Ring-Down Spectroscopy for Detecting and Quantitating Trace Atmospheric Species<br><i>Dr. Richard N. Zare, Stanford University</i> |



**Monday, 18 May 1998 (Cont'd)**

- 11:15 - 11:45 AM      Dynamics of Hypervelocity Collisions at the Gas/Surface Interface  
*Dr. Dennis C. Jacobs, University of Notre Dame*
- 11:45 AM - 12:15 PM      Cluster Ion Beam Deposition for Study of Solid-Solid Interactions  
*Dr. Scott L. Anderson, University of Utah*
- 12:15 - 2:00 PM      *Lunch*
- 2:00 - 2:30 PM      Molecular Beam Studies of Reactions between Stratospheric Gases  
and Supercooled Sulfuric Acid  
*Dr. Gilbert M. Nathanson, University of Wisconsin*
- 2:30 - 3:00 PM      H<sub>2</sub>O Adsorption and Desorption Kinetics on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001)  
*Dr. Steven M. George, University of Colorado*
- 3:00 - 3:30 PM      First Principles Studies of Metal and Metal Oxide Surfaces  
*Dr. Emily A. Carter, University of California*
- 3:30 - 4:00 PM      Efficient Optimization of the Geometries of Large Molecules in  
Internal Coordinates  
*Dr. Peter Pulay, University of Arkansas*
- 7:30 PM      Poster Session

**Tuesday, 19 May 1998**

- 8:45 - 9:15 AM      Rotational and Vibrational Nonequilibrium Effects in Infrared  
Atmospheric Backgrounds  
*Dr. Steven J. Lipson, AFRL, Hanscom AFB*
- 9:15 - 9:45 AM      Gateway Mediated Intersystem Crossing in Acetylene  
*Dr. Robert W. Field, Massachusetts Institute of Technology*
- 9:45 - 10:15 AM      Direct IR Laser Absorption Studies of Radical Kinetics and State-  
To-State Reactive Scattering Dynamics  
*Dr. David J. Nesbitt, University of Colorado*
- 10:15 - 10:45 AM      *Break*
- 10:45 - 11:15 AM      Some Recent Advances in Femtosecond Reaction Dynamics  
*Dr. Ahmed H. Zewail, California Institute of Technology*

**Tuesday, 19 May 1998 (Cont'd)**

- 11:15 - 11:45 AM      Intramolecular Energy Transfer and Bond-Selected  
Photodissociation Dynamics  
*Dr. F. Fleming Crim, University of Wisconsin - Madison*
- 11:45 AM - 12:15 PM      New and Improved Propellants and Propulsion Techniques for  
Rockets and Satellites  
*Dr. Patrick G. Carrick, AFRL, Edwards AFB*
- 12:15 - 2:00 PM      *Lunch*
- 2:00 - 2:30 PM      Cavity Ringdown Laser Absorption Spectroscopy  
*Dr. Richard J. Saykally, University of California, Berkeley*
- 2:30 - 3:00 PM      Vibronic Coherences and The Dissection of Elementary Steps in  
Chemical Dynamics in Condensed Media  
*Dr. V. Ara Apkarian, University of California, Irvine*
- 3:00 - 3:30 PM      Interfacing Electronic Structure Theory with Dynamics  
*Dr. Mark S. Gordon, Iowa State University*
- 3:30 - 4:00 PM      The Generation, Conformations and Energetics of Exotic Species in  
The Gas Phase: Oligomers of Synthetic Polymers and Transition  
Metal Benzene Clusters  
*Dr. Michael T. Bowers, University of California at Santa Barbara*
- 7:30 - 8:00 PM       $I(^2P_{1/2}) + O_2$ : Studies of Low Temperature Electronic Energy  
Transfer and Nuclear Spin State Changing Collisions  
*Dr. Michael C. Heaven, Emory University*
- 8:00 - 8:30 PM      Interactions of HCl( $v=2$ ) with MgO(100)  
*Drs. Curt Wittig and Hanna Reisler,  
University of Southern California*
- 8:30 - 9:00 PM      Surface Scattering of Highly Vibrationally Excited Molecules  
*Dr. Alec Wodtke, University of California at Santa Barbara*

**Wednesday, 20 May 1998**

- 8:30 - 9:00 AM      Optical Excitation, Ionization and Reactive Dynamics of  
Molecular Clusters  
*Dr. Albert W. Castleman, Jr., The Pennsylvania State University*

**Wednesday, 20 May 1998 (Cont'd)**

- |                     |  |
|---------------------|--|
| 9:00 - 9:30 AM      | Spectroscopy and Dynamics in Novel Metal-Containing Clusters<br><i>Dr. Michael A. Duncan, University of Georgia</i>  |
| 9:30 - 10:00 AM     | Linear Scaling Density Functional Methods with Periodic Boundary Conditions<br><i>Dr. Gustavo E. Scuseria, Rice University</i>                             |
| 10:00 - 10:30 AM    | <i>Break</i>   |
| 10:30 - 11:00 AM    | Collective Electronic Excitations in Nonlinear Spectroscopy of Conjugated and Aggregated Molecules<br><i>Dr. Shaul Mukamel, University of Rochester</i>    |
| 11:00 - 11:30 AM    | Two-Color Laser Desorption-Ionization Time-of-Flight Mass Analysis of Aerosols<br><i>Drs. Roger E. Miller and Tomas Baer, University of North Carolina</i> |
| 11:30 AM - 12:00 PM | Vibrational Dynamics in Supercritical Fluids<br><i>Dr. Michael D. Fayer, Stanford University</i>   |
| 12:00 - 12:30 PM    | Ultrafast Vibrational Dynamics in Condensed Phases<br><i>Dr. Dana D. Dlott, University of Illinois at Urbana Champaign</i>                                 |
| 1:00 PM             | BBQ at Hyatt Regency Monterey  |

**1998 High Energy Density Matter Contractor's Meeting  
Naval Postgraduate School and  
Hyatt Regency Monterey  
Monterey, CA  
20-22 May 1998**

**Wednesday, 20 May 1998**

1:00 PM	BBQ at Hyatt Regency Monterey
7:00 PM	Poster Session

**Thursday, 21 May 1998**

7:45 - 8:45 AM	Registration
8:45 - 9:15 AM	Introductory Remarks: <i>Dr. Michael Berman, AFOSR</i>
9:15 - 9:45 AM	Air Force Research Lab Perspective on Advanced Propulsion <i>Dr. Stephen L. Rodgers, AFRL, Edwards AFB</i>
9:45 - 10:15 AM	Solid Parahydrogen <i>Dr. Mario E. Fajardo, AFRL, Edwards AFB</i>
10:15 - 10:45 AM	<i>Break</i>
10:45 - 11:15 AM	Insights into the Stability and Synthesis of High Energy Density Matter through Largescale Computer Simulation <i>Dr. Gregory A. Voth, University of Utah</i>
11:15 - 11:45 AM	Stability and Mobility of O Atoms and Ozone in an Oxygen Matrix <i>Dr. Richard A. Copeland, SRI International</i>
11:45 AM- 12:15 PM	Three-Phase Modeling of Frozen-Ozone Combustion <i>Dr. Martin S. Miller, Army Research Laboratory</i>
12:15 - 2:00 PM	<i>Lunch</i>
2:00 - 2:30 PM	Spectroscopic Characterization of Non-bonding Interactions of the Aluminum Atom <i>Dr. Paul J. Dagdigan, Johns Hopkins University</i>

**Thursday, 21 May 1998 (Cont'd)**

- 2:30 - 3:00 PM            Probing Barriers to the Aggregation of Light Metal Atoms Using Helium Cluster Isolation Spectroscopy  
*Dr. Giacinto Scoles, Princeton University*
- 3:00 - 3:30 PM            Theoretical Investigations of HEDM  
*Dr. Jeffrey A. Sheehy, AFRL, Edwards AFB*
- 3:30 - 4:00 PM            *Break*
- 4:00 - 4:30 PM            Spectral Theory of Adiabatic Electronic Schrödinger Eigenstates: Theory and Implementation for Atomic Aggregates  
*Dr. Peter W. Langhoff, AFRL, Edwards AFB*
- 4:30 - 5:00 PM            Quantitative Analysis of the Condensation of  $B_JC_{n-J}$  Clusters ( $n = 2-12$ ,  $J = 0, 1, 2$ ) in Solid Argon  
*Dr. C. William Larson, AFRL, Edwards AFB*
- 5:00 - 5:30 PM            Advanced Cryogenic Solid Hybrid Rocket Engine Developments for HEDM and Non-HEDM Demonstrations -  
A 1998 Status Report  
*Dr. Eric E. Rice, Orbital Technologies Corporation*

**Friday, 22 May 1998**

- 8:45 - 9:15 AM            Does the  $O_4$  Molecule Exist?  
*Dr. Rodney J. Bartlett, University of Florida*
- 9:15 - 9:45 AM            Extra-High Energy Oxidizers and Fuels  
*Dr. Robert J. Schmitt, SRI International*
- 9:45 - 10:15 AM           An Overview of the FOA Energetic Materials  
*Dr. Henric Östmark, FOA*
- 10:15 - 10:45 AM           *Break*
- 10:45 - 11:15 AM           Reaction Field Cavity Optimization  
*Dr. Teresa Head-Gordon, Lawrence Berkeley National Laboratory*
- 11:15 - 11:45 AM           Potential Energy Surfaces and Dynamics for High Energy Species  
*Dr. Mark S. Gordon, Iowa State University*
- 11:45 AM- 12:15 PM       Fundamental Insights from HEDM Studies  
*Dr. David R. Yarkony, Johns Hopkins University*

**Friday, 22 May 1998 (Cont'd)**

12:15 - 2:00 PM	<i>Lunch</i>
2:00 - 2:30 PM	Development of New Energetic Materials for Advanced Solid Rocket Propellants <i>Dr. Lou Cannizzo, Thiokol Corporation</i>
2:30 - 3:00 PM	Synthesis of High-Energy Density Materials Based on Strained-Ring Compounds <i>Dr. William P. Dailey, University of Pennsylvania</i>
3:00 - 3:30 PM	Theory and Synthesis of New High Energy Density Materials <i>Dr. Karl O. Christe, Raytheon STX</i>
3:30 - 4:00 PM	Pseudochalcogenide Nitrite and Nitrate Analogues <i>Dr. D. Scott Bohle, University of Wyoming</i>
4:00 PM	Closing Remarks, adjourn <i>Dr. Michael Berman, AFOSR</i>

*ITINERARY*  
**Night Operations Working Group Site Visit**  
**437TH AIRLIFT WING CHARLESTON AFB SC**  
*27-29 MAY 1998*

*Current as of 6 May 1998*

**Charleston AFB POC:** Lt. Col. Byron Hepburn  
Office: 803-963-5829  
Home: 803-884-6257

**Billeting:** Charleston AFB Protocol  
Comm: (803) 963-3879 DSN: 673-3879 (Direct Line)

Wednesday, 27 May 1998

**PM Arrival at Leisure/Check in at Charleston House Billeting, Bldg 322**

Thursday, 28 May 1998

0715	<b>Meet in Charleston House (Billeting) Lobby, Bldg # 322 (Lt Col Hepburn and SSgt Pace to greet and pickup visitors)</b>
0730	<b>Continental Breakfast in Support Group Conference Room at Headquarters Bldg</b>
0800-0830	<b>Welcome from Lt Col Hepburn and 437<sup>th</sup> Airlift Wing Vice Commander Colonel Norris Briefings; Team Charleston, C-17, and SOLL II</b>
0830-0900	<b>Circadian and Metabolic Modulation of Human Vision</b> <i>Robert Barlow, Jr., State University of New York</i>
0900-0930	<b>Initiatives from Chronobiology and Circadian Medicine to Maximize Military Readiness</b> <i>Charles A. Czeisler, Brigham and Women's Hospital</i>
0930-1000	<b>New Developments in Identifying the Cumulative Effects of Sleep Restriction</b> <i>David F. Dinges, University of Pennsylvania, School of Medicine</i>
1000-1030	<b>Break</b>

**FOR OFFICIAL USE ONLY**

- 1030-1100    Pharmacological Countermeasures for Physiological Sleepiness: Insights from Pre-Clinic Studies**  
*Dale M. Edgar, Stanford University, School of Medicine*
- 1100-1130    Fatigue and Night Operations**  
*Jonathan French, AL/CFTO, Brooks Air Force Base*
- 1130-1200    Collision Avoidance and Target Engagement**  
*David M. Regan, York University*
- 1200-1300    Lunch at Charleston Club (Buffet)**
- 1315-1415    Tour C-17 Simulator**
- 1430-1515    C-141 SOFI Aircraft Tour (Col Dale Kissinger)**
- 1530-1600    Life Support Visit (Night Vision Goggle Demo)**
- 1615-1715    Free Time**
- 1730           Pickup at Charleston House for dinner with Brig Gen Steve Roser and Mrs. Linda Roser.**  
**Dress: Jacket and Tie for gentlemen, Summer Dress for ladies.**
- 1800           Cocktails at Charleston Place, Downtown in Hospitality Suite 2L**
- 1900-2100    Dinner**

Friday, 29 May 1998
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- 0700-0715    Pickup at Charleston House by Lt Col Hepburn and SSgt Pace (Please checkout prior to departure) Dress: Flight suits for active duty, Casual wear for civilians**
- 0730-0800    Continental Breakfast in DV lounge at the Passenger Terminal**
- 0800           Depart for aircraft**
- 0900-1400    Orientation flight (Box Lunches)**
- 1400-1430    Meeting Wrap Up, DV lounge Passenger Terminal**

**POCs: Lt Col Byron Hepburn, home (803) 884-6257 and SSgt Sharon Pace, office (803) 963-5829**



**AFOSR/ONR/NSF Tribology Program Review**  
**Lowes Annapolis Hotel**  
**Annapolis, MD**  
**22-25 June 1998**

**Monday, 22 June 1998**

- |      |  |
|------|--|
| 0730 | Registration/Continental Breakfast   |
| 0820 | Introduction<br><i>Dr. Hugh De Long, AFOSR, Dr. Peter Schmidt, ONR,<br/>and Dr. Jorn Larsen-Basse</i>  |
| 0830 | Nanotribology, Nanomechanics and New Molecular Probes<br><i>Charles M. Lieber, Harvard University</i>  |
| 0900 | Solid Lubricant Replenishment Systems<br><i>Thierry A. Blanchet, Rensselaer Polytechnic Institute</i>  |
| 0930 | Design of Tribological Properties via Self-Assembling<br>Nanocomposite Molecular Films<br><i>Vladimir V. Tsukruk, Western Michigan University</i>              |
| 1000 | <i>Break</i>   |
| 1015 | Nanotribological Studies of Bulk Ceramic Materials,<br>Multilayered Thin Films, and Liquid Lubricant Films<br><i>Bharat Bhushan, The Ohio State University</i> |
| 1045 | Surface Treatments for Probing of Tribological State Variables,<br><i>Ursula Gibson, Dartmouth College</i>   |
| 1115 | Theoretical Simulations of Low-Dimensional Materials<br><i>J. W. Mintmire, C. T. White, Naval Research Laboratory</i>  |
| 1145 | Friction Control in Thin Film Lubrication<br><i>Jianping Gao, W. D. Luedtke, <u>Uzi Landman</u>,<br/>Georgia Institute of Technology</i>                       |
| 1215 | <i>Lunch</i>   |

**Monday, 22 June 1998 (Cont'd)**

- 1400                    Magnetron Sputtered Quasicrystalline Coatings - A Breakthrough for Thin Film Applications  
*Larry L. Fehrenbacher, Technology Assessment & Transfer, Inc.*
- 1425                    Tribological Behavior of Sputtered Quasicrystalline Alloys in Extreme Environments - - A Preliminary Study  
*Michael N. Gardos, Raytheon Systems Company*
- 1450                    Frictional Properties of Quasicrystalline Surface  
*Andrew J. Gellman, Carnegie Mellon University*
- 1515                    Investigation of Quasicrystal Coatings for Friction and Wear Control in Extreme Environments  
*J. S. Zabinski, N. A. Pierce, S. V. Prasad, AFRL/MLBT*
- 1540                    *Break*
- 1555                    The Surface Chemistry and Tribology of Metal Carbides and Nitrides  
*Scott S. Perry, University of Houston, Steve Didziulis, The Aerospace Corporation*
- 1625                    Preparation of Carbon Films on SiC by High Temperature Chlorination  
*M. McNallan, D. Ersoy, Y. Gogotsi, University of Illinois at Chicago*

**Tuesday, 23 June 1998**

- 0730                    Continental Breakfast
- 0830                    Kelvin Probe Measurements Applied to Bearing Diagnostics  
*Steven Danyluk, YeYuan Yang, Georgia Institute of Technology*
- 0900                    Sliding Friction and Wear of Selected Aluminum-Based Bearing Alloys and Preliminary Results Using an *In Situ* Kelvin Probe to Monitor Changes in Surface Condition  
*K. Lepper, J. Chashechkina, T. Kasai, A. Zharin, and D. A. Rigney, The Ohio State University*
- 0930                    Mixing of Materials During Sliding with and Without Lubrication  
*John L. Young, Jr., D. Kuhlmann-Wilsdorf, and Robert Hull, University of Virginia*

**Tuesday, 23 June 1998 (Cont'd)**

- 1000                    *Break*
- 1015                    Debris Denting, Spall Initiation and Propagation in Lubricated Contacts  
*Farshid Sadeghi, Purdue University*
- 1045                    Deformation Behavior of Thin Liquid Films at Elevated Pressure  
*Scott Bair, Georgia Institute of Technology*
- 1115                    Transient Behavior of Rotary Lip Seals  
*Richard F. Salant, Georgia Institute of Technology*
- 1145                    Recent Advances in Experimental Techniques for Investigating High  
Speed Friction  
*Vikas Prakash, Case Western Reserve University*
- 1215                    *Lunch*
- 1400                    Spectroscopic Probes of Boundary Lubricants and Perfluoropolyethers  
*Steve Granick, University of Illinois*
- 1430                    *In Situ* Laser Spectroscopic Studies of Boundary Lubricant Films  
*Gerold A. Willing, Sangkwon Park, Ronald D. Neuman,  
Auburn University*
- 1500                    Characterization of Surface Reactions on Iron in the Presence of  
Perfluoropolyalkylether Lubricants at Elevated Temperatures  
*Jeffrey H. Sanders, AFRL MLBT*
- 1530                    *Break*
- 1545                    Tribological Surface Chemistry  
*Andrew J. Gellman, Carnegie Mellon University*
- 1615                    Free Vibration Analysis of PZT Glide Heads during Disk/Head  
Interfacial Contacts  
*Alex Y. Tsay, I. Y. (Steve) Shen, University of Washington,  
C.-P. Roger Ku, IBM, Bruno Marchon, Seagate Technology*
- 1645                    Structural Analysis of MEMS Pressure Sensors for Disk/Head  
Interfacial Contact Application  
*Liwei Lin, Yen-Wen Lu, The University of Michigan*

**Wednesday, 24 June 1998**

- 0730 Continental Breakfast
- 0830 Lubricative Gas-Phase Reactions of Silicon and Polycrystalline Diamond with Dry/Wet Hydrogen and Dry Oxygen for MEMS Applications  
*Michael N. Gardos, Raytheon Systems Company*
- 0900 Development of a New, Reactive Potential Energy Function to Study the Tribology of Hydrocarbon Systems  
*Judith A. Harrison, United States Naval Academy*
- 0930 Nano-Composite Coatings Consisting of Carbides, Diamond-Like Carbon, and Dichalcogenates for Aerospace Tribology  
*A. A. Voevodin, J. P. O'Neill, J. S. Zabinski, AFRL MLBT*
- 1000 Break
- 1015 Nanotribology of Vapor-Phase Lubricants  
*Jacqueline Krim, North Carolina State University*
- 1045 Vapor Lubrication Mechanisms: Heat Generation in High Speed Rolling Element Bearings  
*Nelson H. Forster, Lewis Rosado, Garry D. Givan, AFRL PRSL*
- 1115 Studies of the Effect of PVD TiN Coatings on the Rolling Contact Fatigue Life  
*L. M. Keer and Y.-W. Chung, Northwestern University*
- 1145 Thermal-Tribological Designs of Mechanical Elements  
*Qian (Jane) Wang and Y. Cao, Florida International University*
- 1215 Lunch
- 1400 *In Vivo* Raman Tribometry: Real-time Analysis of Friction, Wear and Third Body Processes  
*I. L. Singer, K. J. Wahl, Naval Research Laboratory*
- 1430 Sol-Gel Derived, Nanostructure Dioxide Lubricant Coatings  
*Douglas J. Taylor, Stuart T. Schwab, Patrick F. Fleig, TPL, Incorporated, Richard A. Page, Southwest Research Institute*

**Wednesday, 24 June 1998 (Cont'd)**

- 1500            *In Situ* Studies of the Nucleation and Growth of Cubic Boron Nitride  
L. D. Marks, E. Bengu, C. Collazo-Davila, Northwestern University
- 1530            *Break*
- 1545            Atomistic Simulations of Adhesive Interactions with  $\alpha$ -Alumina and  
Hydroxylated  $\alpha$ -Alumina Surfaces  
William L. Hase, Wayne State University
- 1615            Friction and Adhesion Studies Using the Surface Forces Apparatus  
Jacob Israelachvili, Cyrus Safinya, Yuval Golan,  
University of California at Santa Barbara
- 1645            Adhesion studies: Liquid Capillarity and Micro-scale Impact  
Dr. Jeffrey L. Streator, Georgia Institute of Technology

**Thursday, 25 June 1998**

- 0730            Continental Breakfast
- 0830            Predicting Fracture Behavior of Polycrystalline Covalent Ceramics  
Using a Hybrid of Computational Methods  
Donald W. Brenner, Olga A. Shenderova, North Carolina State University
- 0900            Adaptive Wide Temperature Solid Lubricant Films by Magnetron  
Sputtering and Ion Beam Assisted Deposition  
Larry L. Fehrenbacher, Technology Assessment Transfer, Inc.
- 0930            Lubrication Mechanisms in Zinc Oxide Coatings  
J. S. Zabinski, N. Pierce, J. Nainaparampil, S. V. Prasad, AFRL MLBT
- 1000            *Break*
- 1015            Modeling the Interactions Between Compressed Polymer Surfaces  
Anna C. Balazs, University of Pittsburgh
- 1045            *In Situ* Investigation of the Influence of a Mechanical Load on the  
Orientation of Organic Monolayers with Second Harmonic Generation  
F. Eisert, M. Gurka, M. Buck, and M. Grunze,  
Institut für Angewandte Physikalische Chemie

**Thursday, 25 June 1998 (Cont'd)**

- 1115                    A Robust, Deterministic Model for Thermal Mixed-Film Lubrication  
*Liming Chang, Penn State University*
- 1145                    The Nature of Tribochemistry & It's Effect on Lubrication  
*Stephen Hsu, University of Maryland/(NIST)*
- 1215                    *Lunch*
- 1400                    An Investigation of Certain Dynamic Instabilities in Dry Sliding  
*George G. Adams, Northeastern University*
- 1430                    Density-Functional Chemical Dynamics with Fractional  
Occupation Numbers,  
*Brett I. Dunlap, Naval Research Laboratory*
- 1500                    An Integrated Study on Conformal Contacts  
*Qian (Jane) Wang, Florida International University*
- 1530                    *Break*
- 1545                    Integrated Diagnostics  
*Richard S. Cowan, Georgia Institute of Technology*
- 1615                    Chemical Imaging and Molecular Diagnostics Using  
Optical Spectroscopy  
*Dor Ben-Amotz, Purdue University*
- 1645                    Modeling of Lubrication Breakdown of Sliding Contacts  
*Dr. Si. C. Lee, The Ohio State University*

## Agenda

### Mechanism of Al Alloy Corrosion and the Role of Chromate Inhibitors MURI Program Review

January 11-12, 1999

Monday, January 11, 1999

- |               |  |
|---------------|--|
| 9:00 - 9:30   | Overview (Frankel)   |
| 9:30 - 10:30  | Surface Science Aspects of Chromate Inhibition<br>(Clayton/Halada)                               |
| 10:30 - 10:45 | break  |
| 10:45 - 11:45 | XANES and Electrochemical Studies of Chromate Conversion<br>Coatings and Pure Aluminum, (Isaacs) |
| 11:45 - 1:00  | lunch  |
| 1:00 - 2:00   | Chromate Inhibitors in Paint Systems (Granata)   |
| 2:00 - 3:00   | Filiform Corrosion of Al Alloys (Stratmann)  |

Tuesday, January 12, 1999

- |               |   |
|---------------|---|
| 9:00 - 10:00  | Structure and Dynamics of Chromate Films on AA2024-T3<br>(McCreery)   |
| 10:00 - 10:30 | break   |
| 10:30 - 11:30 | The Effect of Chromate on Localized Dissolution of Alloys<br>(Frankel)  |
| 11:30 - 1:00  | lunch   |
| 1:00 - 2:00   | Mechanism of Al Alloy Corrosion and the Role of Chromate<br>Inhibitors – Ionic and Intermetallic Aspects (Kendig) |
| 2:00 - 3:00   | Summary (Frankel)   |

## **Agenda**

### **MURI: Prevention of Corrosion in Structural Aluminum Alloys**

**Wednesday, January 13, 1999**

#### **Morning session: 9:00am - 11:30 am**

9:00 am

"Prevention of Corrosion in Structural Aluminum Alloys"

K. Sieradzki, *Arizona State University*

9:40 am

"Corrosion-Induced Nanostructure and Morphology of Aluminum Alloys"

R. Carpenter, *Arizona State University*

Break 10:20 am - 10:35 am

10:40 am

"Electrochemistry of Cu Redistribution During Corrosion of Aluminum Alloys"

N. Dimitrov, *Arizona State University*

Lunch 11:30 am - 12:55 pm

#### **Afternoon session 1:00 pm - 3:00 pm**

1:00 pm

"Mechanisms of particle removal and copper redistribution on 2024 surfaces"

A. Davenport, *Univ. of Manchester/Univ. of Birmingham*

1:40 pm

Computer Simulations of Aluminum Alloy Corrosion

J. Erlebacher, *Harvard Univ.*

2:20 pm

Protecting Aluminum Alloys Against Copper: The Future

R. Newman, *UMIST*





AGENDA FOR JANUARY 14, 1999  
URI REVIEW – North Dakota State University

<u>TIME</u>	<u>TOPIC</u>	<u>SPEAKER</u>
9:00	Introduction & Project Summary	Gordon Bierwagen
9:20	Improved EIS Instrumentation Design	David Farden
10:30	BREAK	
10:50	Sample Handling & Electrochemical Data	Gordon Bierwagen
11:30	AFM Results & Implications	Dennis Tallman
12:00	LUNCH	
12:45 PM	SVET & Conductive Polymer Results and Interpretation	Dennis Tallman
1:15	Spectroscopic Results & Interpretation	Marek Urban
2:30	Conclusions and Future Work	Gordon Bierwagen

**1999 Durable Coatings Program Review  
Hawk's Cay Resort and Marina  
Osprey Room  
Duck Key, Florida  
15 January 1999**

**Friday, 15 January 1999**

7:25 - 8:25 AM	Registration/Continental Breakfast
8:25 - 8:30 AM	Introductory Remarks <i>Dr. Charles Lee, AFOSR</i>
8:30 - 9:15 AM	UniCoat Airplane Coatings System: Corrosion Resistant Ceramer Coatings <i>Dr. Mark D. Soucek, North Dakota State University</i>
9:15 - 10:00 AM	Durable Multilayer Coatings <i>Dr. Thomas Seery and Dr. Jeff Koberstein, University of Connecticut</i>
10:00 - 10:15 AM	<i>Break</i>
10:15 - 11:00 AM	Characterization of Heterogeneous Regions in Polymer Coatings <i>Dr. Dharmaraj Raghavan, Howard University</i>
11:00 AM - 12:00 PM	Characterization of Aging-Induced Physical and Chemical Defects in Aircraft Long-Life Coating Systems <i>Dr. Y. C. Jerry Jean and Dr. Thomas C. Sandreczki, University of Missouri-Kansas City</i>
12:00 - 1:30 PM	<i>Lunch</i>
1:30 - 2:15 PM	Optical Imaging for Nondestructive Evaluation of Microstructure, Fracture, Delamination and Degradation in Multilayer Organic Coatings and Paints <i>Dr. Paras N. Prasad, State University of New York at Buffalo</i>
2:15 - 2:45 PM	Multi-Color Electrochromic Polymer Coatings <i>Dr. John R. Reynolds, University of Florida</i>
2:45 - 3:00 PM	<i>Break</i>

**Friday, 15 January 1999 (Cont'd)**

3:00 - 3:30 PM	Corrosion Protection of Aluminum and Aluminum Alloys Using Polyanilines <i>Dr. Arthur J. Epstein, The Ohio State University</i>
3:30 - 4:30 PM	Coating Technology for Long Term Air Force Goals <i>Dr. Fred E. Arnold, AFRL MLBP, WPAFB</i>
4:30 PM	Adjourn

# ≈ AGENDA ≈

## NDE-MURI Review 1999

January 18 - 19, 1999

Location: Hawk's Cay Resort  
Duck Key, Florida

### Monday, January 18, 1999

#### Overview

9:00 – 10:00 A.M. Overview of the NDE-MURI Program (Matikas)

#### Quantification of LCF/HCF Damage

10:00 – 10:15 A.M. Characterization of Fatigue Damage Accumulation (Maurer)  
10:15 – 10:30 A.M. **BREAK**  
10:30 – 11:00 A.M. Real - Time Monitoring of Fatigue Damage through Nonlinear Acoustics (Sathish)  
11:00 – 11:30 A.M. LCF/HCF Interaction Using a 20 kHz HCF Cell (Matikas)  
11:30 – 1:00 P.M. **LUNCH**  
1:00 – 1:15 A.M. Temperature Monitoring of Fatigue Damage (Meyendorf)  
1:15 – 2:00 P.M. Early Detection of Fatigue Cracks – Eddy Current and Laser-Ultrasonic Techniques (Nagy)  
2:00 – 2:30 P.M. Fatigue Crack Detection via Holography and Interferometry of SAW (Blackshire)  
2:30 – 2:50 P.M. Image Processing for Phase-Stepped Interferometry and Resolution Enhancement (Hardie)  
2:50 – 3:00 P.M. Summary and Concluding Remarks  
3:00 P.M. Adjourn

### Tuesday, January 19, 1999

#### Fretting Fatigue Damage Characterization

9:00 – 9:30 A.M. Prediction of Fatigue Crack Instability through Surface Nondestructive Characterization (Matikas)  
9:30 – 10:00 A.M. Interface Contact Conditions in Fretting Fatigue - Fretting Maps and Temperature Rise (Nicolaou)  
10:00 – 10:30 A.M. **BREAK**  
10:30 – 10:45 A.M. Nano-scale NDE for Elastic Property Imaging (Sathish)  
10:45 – 11:15 A.M. Characterization of Fretting Fatigue Damage on Ti-6Al-4V Alloys (Nicolaou)  
11:15 – 1:00 P.M. **LUNCH**

#### Corrosion Characterization

1:00 – 1:45 P.M. Pitting Initiation and Coating Degradation – Developing Corrosion and NDE Metrics (Khobaib)  
1:45 – 2:30 P.M. Microradiographic Detection of Corrosion (Rokhlin)  
2:30 – 2:45 A.M. NDE of Protective Coatings (Meyendorf)  
2:45 – 3:00 P.M. Summary and Concluding Remarks  
3:00 P.M. Adjourn

**Agenda**  
**3<sup>rd</sup> Annual Review of AFOSR MURI**  
**"Nanoscale Devices and Novel Engineered Materials"**  
**University of Florida**  
**Monitor: Maj. H.C. DeLong, Ph.D.**

**Wednesday**

**January 20, 1999**

**Location: Hawk's Cay Resort, Marathon, FL**

9:00-9:20 am      Welcome and Overview; Program Goals and Achievements  
S.J. Pearton (MSE/UF)

**Novel Engineered Materials and Properties**

9:20-10:00 am      Mechanical Properties of Nanostructured Materials  
S.A. Syed Asif (NRL)  
10:00-10:30 am      Nanostructured Display Materials, P.H. Holloway (MSE/UF)  
10:30-11:00 am      Coffee Break

**New Directions**

11:00-11:15 am      Magnetotransport – charge, frequency and noise properties  
A.F. Hebard (Physics/UF)  
11:15-11:30 am      Integration of Magnetic Materials and Semiconductors  
F. Ren (Chem. Eng./UF)  
11:30-12:00 am      Deposition and Etching of Ferromagnetic Particles in a Non Magnetic  
Matrix, A.C. Kummel (Chem/UCSD)  
12:00-1:30pm      Lunch  
1:30-2:00 pm      Pulsed Laser Deposition of CMR Oxides, R.K. Singh (MSE/UF)  
2:00-3:00 pm      Discussion (all)

**Thursday**

**January 21, 1999**

**Submicron Magnetic Structures: Deposition, Processing and Theory**

9:00-9:15 am      Overview and Accomplishments, S.J. Pearton (MSE/UF)  
9:15-10:00 am      Physics of Length Scales in Magnetic and Superconducting  
Microstructures, I.K. Schuller (Physics/UCSD)  
10:00-10:30 am      Integration of Magnetic Nanoparticles with 2-D Electron Systems  
S. von Molnar (Physics/FSU)  
10:30-11:00 am      Coffee Break  
11:00-11:30 am      Nanostructure Patterning and Transport Physics  
F. Sharifi (Physics/UF)  
11:30-12:00 am      Ion Beam Deposited GMR Materials  
D. Temple and G.E. McGuire (MCNC)  
12:00-1:30 pm      Lunch  
1:30-2:00 am      Dry Etching of Magnetic Multilayers, S.J. Pearton (MSE/UF)  
2:00-2:30 pm      Theory and Modelling of GMR, S. Hershfield (Physics/UF)  
2:30-2:45 pm      Summary/Accomplishments, S.J. Pearton  
2:45-3:30 pm      Discussion (all)

**AFOSR STTR PROGRAM REVIEW**  
18-19 February 1999

Holiday Inn Conference Center I-675  
Patterson Room  
Fairborn, Ohio

Thursday, 18 February (Adhesives)

- 0800 AdTech - Dielectric Relaxation Spectroscopy of Adhesively Bonded Joints
- 0840 Aspen Systems - Liquid Crystalline Adhesive with Zero Shrinkage
- 0920 Cornerstone - High-Performance Liquid Crystal Adhesives
- 1000 Break
- 1015 DACCO - Electrochemical Sensors for Nondestructive Evaluation of Adhesive Bonds
- 1055 PolyComp - Development of High Temperature Low Cure Shrinkage Adhesives
- 1135 Triton - High Temperature Low Viscosity Polyimide Adhesive
- 1215 End

Friday, 19 February 1999 (Flexible Electronics and Photonics)

- 0830 AdTech - Flexible Electronics and Photonics
- 910 Materials Research Institute - Inkjet Printing of Flexible Circuits on Polymer Substrate
- 0950 Break
- 1010 Pacific Wave Inc. - Flexible Polymer Modulators for Large Conformal Antenna Arrays
- 1050 UNIAX - Polymer LEDs made from Monochromatic Red-Emitting Polymer/Rare Earth Blends
- 1130 End